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DEPARTMENT OF PHYSICS
SCHOOL OF SCIENCES AND HEALTH PROFESSIONS
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA

Technical Report PTR-82-5

SCIENCE AND SOFTWARE SUPPORT FOR SPACECRAFT
SOLAR OCCULTATION EXPERIMENTS

By

Ghiassi-Hessameddin

and

Jacob Becher, Principal Investigator

Final Report
For the period ending September 1979

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

Under
Research Contract NSG-1341
Michael P. McCormick, Technical Monitor
Instrument Research Division
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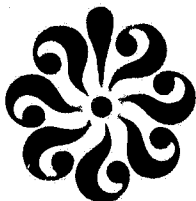

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SCIENCE AND SOFTWARE SUPPORT FOR SPACECRAFT SOLAR OCCULTATION EXPERIMENTS

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Ghiassi-Hessameddin*

ABSTRACT

The temperature dependence of absorption coefficients of ozone was studied between 7567 Å and 4630 Å. When the gas was cooled from room temperature to -108° C, an overall increase in the absorption coefficients was noticed. The maximum increase of 5% occurred at $\lambda = 6020$ Å. In general, the absorption is linearly dependent on temperature.

INTRODUCTION

Ozone is one of the simplest triatomic molecules. Its importance in atmospheric chemistry has been the main reason for the sustained interest in its spectrum and molecular structure. A uniform and consistent set of ozone absorption coefficients is highly desirable since such data are important in atmospheric monitoring and quantitative ozone technology (such as rocket propulsion, water purification, disinfection, sterilization of containers for food, and sterilization of sewage). A number of basic research projects during the last decade have supplied new data and expanded the knowledge of the absorption spectrum.

Ozone has absorption bands extending from the infrared and visible to the ultraviolet (UV). The infrared regions' bands, which have been extensively studied, start at 3.3 μm and extend to 14.3 μm, with the strongest at 9.6 μm. The UV absorption spectrum consists of three bands: Chalonge

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Lefebvre band (3400 Å to 3650 Å); Huggins band (3050 Å to 3400 Å); and Hartley band (2200 Å to 3000 Å). The strongest and most featureless absorption in UV is the Hartley band with a maximum at 2550 Å, filtering most of the incoming radiation to the atmosphere that would otherwise reach the earth's surface. The Huggins band is a weak band with well-defined features that are further enhanced by lowering the gas temperature. The weakest is the Chalonge Lefebvre band with known features, similar to Huggins bands, that increase in prominence by decreasing the temperature. The only band in the visible is the Chappuis band--a very weak band with a maximum of 6020 Å with few apparent features. This band is used for monitoring concentrations of atmospheric ozone, even though the absorption coefficients in UV are better known. Other visible atmospheric absorption measurements for ozone are preferred because of the simplicity in experimental design and operation of the apparatus. Of the five studies (refs. 1-5) of absorption of coefficients in the visible region, only two agree substantially (refs. 3 and 4). The others reported that the magnitude of the absorption coefficients differed by about 10%. The major disagreement surrounds the conclusion reported on the temperature dependence of the absorption coefficient. This controversy was the motivation for doing this research.

The weakness of the absorption in the visible region requires spectroscopic measurements to be made with a cell containing a high concentration of the gas. The technique to obtain highly concentrated ozone has made it necessary to produce pure liquid ozone and then boil the liquid for transferring the ozone into the absorption cell. This is particularly dangerous since the slightest vibration could cause an exothermic reaction that could result in a serious explosion. This potential hazard may account for the fact that many important physical properties of this substance are not accurately known. The usual techniques for determining physical properties can rarely be applied; contact with materials usually used in experimental work must be avoided. Experience has shown that the most satisfactory materials for construction of the vacuum system are glass and teflon, which have been used in this work.

REVIEW OF PREVIOUS RESEARCH

Absorption Coefficients

The absorption coefficients of ozone in the visible region have been the subject of numerous studies (refs. 1-5). Early experiments used ozonized oxygen whereas those performed later by Inn and Tanaka (ref. 4) and Griggs (ref. 5) used pure ozone. The measurements performed with ozonized oxygen relied on a separate measurement of the composition; thus, the early measurements of absorption were limited by the effectiveness of determining the compositions of the two measurements. These compositions would vary over the time of the experiment, since a small amount of impurities and concentration of O_3 are the determining factor of O_3-decomposition rate. In view of the weakness of the Chappuis absorption, high concentrations of the gas are required in the optical path to set a detectable signal. Thus, the researcher who used a mixture of ozone and oxygen had to use a long path to compensate for the oxygen in the tube. The concentration in the cell was determined either chemically or by observing the UV spectrum. The pressure measurements in the absorption tube were determined using a H_2SO_4 manometer. This type of manometer has a vapor pressure which introduces impurities into the gas sample, affecting the decomposition rate of O_3. Pure ozone absorption measurements of the Chappuis band by Inn and Tanaka were the results of an interpolation dependent on O_3 decomposition. The spectrum they measured was corrected by observing the decay of ozone which was monitored at a fixed wavelength using a gas cell at the same temperature and pressure. They reported a decay of about 12% in a five- to ten-minute interval. Later, Griggs purified ozone to 100% and was unable to detect any decay, yet he confirmed the findings of Inn and Tanaka in UV. However, in the visible region his measurements seem to agree better with the previous work by Vigroux (ref. 3).

Temperature Dependence of Absorption Coefficients

In 1882 Chappuis, who two years earlier discovered the band that now bears his name, was the first to report the influence of temperature on the

temperature on the absorption coefficient (ref. 6). The mixture he used to perform measurements in the range from room temperature to -50° C contained 5% ozone. In 1935 Lefebvre (ref. 7) found the absorption spectrum in this region to be exactly the same at -80° C and room temperature using a mixture containing 6% ozone. Later, the variation in absorption coefficients was reported by Vassy (ref. 8), who had used a more concentrated mixture of ozonized oxygen containing 60-70% ozone. His values for absorption were about 20% higher than those reported earlier. He found a variation of nearly 30% for the temperature range of 18° C to -105° C. In 1947, Humphrey and Badger (ref. 9), used a mixture of 6% ozone and found no significant change in the absorption coefficients from room to dry ice temperatures. Later in 1948, Vassy and Vassy (ref. 2) investigated their previous findings, and corrected the error in the wavelengths they reported but confirmed the temperature dependence. Finally in 1953 Vigroux (ref. 3) measured the absorption coefficients and temperature effects for all three ranges (infrared, visible, and UV). He established new values for the absorption coefficient in the visible region with peak of absorption of 0.059 cm^{-1} (base 10) at λ = 6020 Å using an ozone concentration of approximately 30%. He employed a cross-shaped absorption tube, one arm of which was always used to determine the concentration of ozone by monitoring the UV band. Consequently, he was able to obtain the reduced thickness. Concerning temperature dependence, Vigroux supported the results of Humphrey and Badger. It should be noted that the determination of impurities and spectral data were not performed simultaneously. Inn and Tanaka (ref. 4) conjectured that a systematic error existed in Vassy's method of measuring the reduced thickness of ozone, and that the error could account for the large discrepancies between Vassy's findings and those of later researchers.

All the temperature effect measurements were performed photographically. The researchers had to cope with the problem of thermal equilibrium in the absorption cell at low temperatures. To avoid condensation of moisture on cell windows, pure air was blown on both ends of the cell. This moving dry air caused some heat exchange through the windows between the ozone molecules.

CHARACTERISTICS OF OZONE

Appropriate handling of ozone requires some knowledge of its physical and chemical properties. This knowledge is particularly important in the processes of purification and variation of temperature.

Physical Properties of Ozone

The following physical properties of ozone were important for our experiment and its spectral analysis:

A. Ozone is a blue gas with a characteristic odor (ref. 10). The boiling and melting points of pure ozone are $-111.9°$ C (ref. 11) and $-192.5°$ C (ref. 12) respectively. The binding energy for ozone is 1.04 eV (ref. 13). This small value is indicative of the reactivity and oxidizing characteristics of this molecule.

B. The ozone molecule O_3 is an isosceles triangle belonging to symmetry group C_2v (i.e., a two-fold symmetry axis and two planes of symmetry containing this axis). In this point group there are four types of electronic states which, according to Herzberg (ref. 13), are classified as A_1, A_2, B_1, B_2 (Table 1). Taking into account the electron spins and the rotational motion of the molecule (which produce a magnetic field), the four electronic states are split into eight components (four singlets and four triplets).

Table 1. Character table of the symmetry group C_2v.

C_{2v}	I	$C_2(z)$	$\sigma_v(yz)$	$\sigma_v(xz)$
A_1	+1	+1	+1	+1
A_2	+1	+1	-1	-1
B_1	+1	-1	+1	-1
B_2	+1	-1	-1	+1

The description of electronic states in polyatomic molecules such as ozone depends largely on the method of calculation. Among the variety of approaches (such as MO, HF, LCAO-SCF, VB, SCVMO, and GVB) used to provide a description and calculation of electronic states, the method of generalized valence bond (GVB) leads to a firm conceptual model for understanding the nature of ozone's molecular states. In addition, the GVB method is based on rigorous quantum mechanical considerations using high-speed digital computers for calculation of the electronic wave functions. The emphasis here is to introduce concepts that make it easier to visualize electron configurations without doing specific calculations. The GVB model assigns an orbital for each electron (each pair consists of two highly overlapping orbitals). The orbitals are often localized onto centers different from their atomic origins. The description of molecules in the GVB approach requires an understanding of chemical bonding principles which, briefly stated, are as follows: In order to obtain a strong covalent bond between atoms it is essential that (1) a singly occupied orbital on each atom be such that it overlaps significantly when the atoms are brought together, and (2) the orbitals of the bond must be nearly orthogonal to the other orbitals of the molecule not involved in the bond.

In order to apply the GVB approach for O_3 (ref. 14) we first examined the atomic orbitals of O, O_2, and, finally, O_3. The usual orbitals for oxygen are $(1s)^2$, $(2s)^2$, $(2p)^4$ with doubly occupied 1s, 2s, 2p(p_x) and two singly occupied 2p(p_y), 2p(p_z) orbitals. Taking two oxygen atoms, there are two ways to couple the p orbitals. (Molecular orbitals that arise from p atomic orbitals are often called π orbitals.) Case A (Figure 1) shows a doubly occupied p_x orbital belonging to the right atom combined with a singly occupied p_x of the left atom and a singly occupied orbital (p_y) on the right atom with a doubly occupied orbital (p_y) on the left atom. In p_x orbital combination, the energy of the singly occupied p_x orbital of the left oxygen atom increases as the interatomic distance R decreases (antibonding character) leading to the orthogonalization between the double- and single-occupied orbitals. Furthermore, the double-occupied p_x orbital diminishes its electron-electron interaction by delocalizing onto the left oxygen atom decreasing the shielding of the left nucleus. The interaction produced by these three electrons

leads to a binding energy of about 30 kcal. The same situation exists for the p_y orbitals leading to the same energy. Thus, total bonding for O_2 would be about 60 kcal. In case B, the two singly occupied p_x of each oxygen are combined to form a doubly occupied, high overlapping orbital. This brings the p_y orbitals together, acquiring antibonding character in order to be orthogonal to each other. The increased antibonding in case B compared to case A makes it reasonable to expect case A to be more stable (ground state). Similar to cases A and B, the third oxygen atom can be combined in two ways to one of the O in O_2. (These configurations are classified by the numbers of electrons in π orbitals.) One can easily conclude that π^4 configuration is more stable than π^5; therefore, it is the ground state (O_3). The manifold of electronic states of ozone can be obtained from π^4 (ground state) by exciting an elecron in a doubly occupied p orbital (in the plane) of O to a singly occupied orbital (perpendicular to the plane of the molecule). This results in a π^5 electronic state with two equivalent configurations (Figure 1). This in turn leads to two singlet and two triplet states. Again, by exciting an electron from the doubly occupied p orbital (in the plane) of O to the singly occupied (perpendicular to the plane), π^6 configuration appears with two states ($2^1A_1, {}^3B_2$). In the 2^1A_1 state the singly occupied orbitals (in the plane with spins of -1/2 and +1/2) can bond together yielding to an energy of about 1.5 eV above the ground state. Other states of ozone can be obtained by taking the most loosely bound electrons to various higher orbitals. Figure 2 shows the energies of different configurations of ozone based on theoretical calculations.

All of these predicted states have bond angles (ref. 15) ranging from 100 degrees to 120 degrees (Figure 3) with the exception of state 2^1A_1 which has an angle of 60 degrees (ring ozone). Transitions between states of ozone have been identified (refs. 16-19) as ${}^3B_2 \longleftarrow {}^1A_1$ for infrared, ${}^1B_2 \longleftarrow {}^1A_1$ for Hartley band, and as a blend of transitions for Chappuis region, (${}^1B_1 \longleftarrow {}^1A_1$ and ${}^1A_2 \longleftarrow {}^1A_1$). There is no consensus for Huggins band though it has been suggested (refs. 20 and 21) that it could belong to the same transition as Hartley band.

Chemical Properties of Ozone

The decomposition of ozone is extremely complex and difficult to study. Although the decomposition of the gaseous phase has been the subject of extensive research, no satisfactory mechanism has ever been suggested to explain either the thermal or photochemical decompositions. Most of the known results indicate that the thermal decomposition is a result of the following mechanism:

$$M + O_3 \underset{2}{\overset{1}{\rightleftharpoons}} O_2 + O + M$$

$$O + O_3 \xrightarrow{3} 2O_2$$
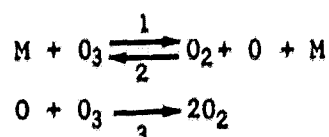
Reaction 2 is much faster than reaction 3 where M may be an inert molecule (such as O_2, N_2, CO_2, He). The relative efficiencies depend on the particular gas M in activating O_3 (compared to O_3 itself). The effectiveness of the reactions 1 and 2 are: O_2 = 0.44, N_2 = 0.41, CO_2 = 1.06, and He = 0.34 compared to O_3 = 1.00. The rate constants for reactions 1 through 3 are as follows (ref. 22):

$$k_1 = 4.61 \times 10^{12} \exp(-24000/RT) \text{ liter/(mole} \times \text{sec.)} \tag{1}$$

$$k_2 = 6.00 \times 10^{7} \exp(+600/RT) \text{ liter}^2/(\text{mole}^2 \times \text{sec.)} \tag{2}$$

$$k_3 = 2.96 \times 10^{10} \exp(-6000/RT) \text{ liter/(mole} \times \text{sec.)} \tag{3}$$

where R is universal gas constant in cal/moles. The specific rate constants of equations 1-3 are k_1, k_2, k_3. The atomic oxygen reaction rates for the mechanism 1-3 are:

$$+\left(\frac{d[O]}{dt}\right)_1 = k_1[M][O_3] \tag{4}$$

$$-\left(\frac{d[O]}{dt}\right)_2 = k_2[O_2][O][M] \tag{5}$$

$$-\left(\frac{d[O]}{dt}\right)_3 = k_3[O][O_3] \tag{6}$$

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Assuming a stationary state for atomic oxygen, it follows that:

$$+\left(d[O]_{ss}/dt\right)_1 - \left(d[O]_{ss}/dt\right)_2 - \left(d[O]_{ss}/dt\right)_3$$

Substituting equations 4, 5, and 6 into equation 7 we obtain:

$$k_1[O_3][M] = k_2[O_2][M][O]_{ss} + k_3[O]_{ss}[O_3] \tag{7}$$

solving the above equation for $[O]_{ss}$ we get equation 8:

$$[O]_{ss} = \frac{k_1[O_3][M]}{k_2[O_2][M] + k_3[O_3]} \tag{8}$$

In order to obtain the reaction rates for O_3 while atomic oxygen is in equilibrium, we can write from mechanisms 1, 2, and 3 the following rate equations:

$$-\left(\frac{d[O_3]}{dt}\right)_1 = k_1[M][O_3] \tag{9}$$

$$+\left(\frac{d[O_2]}{dt}\right)_2 = k_2[O_2][O]_{ss}[M] \tag{10}$$

$$-\left(\frac{d[O_3]}{dt}\right)_3 = k_3[O]_{ss}[O_3] \tag{11}$$

Thus

$$-\left(\frac{d[O_3]}{dt}\right)_{total} = k_1[M][O_3] - k_2[O_2][O]_{ss}[M] + k_3[O]_{ss}[O_3] \tag{12}$$

Using equations (8) and (12) we obtain for the decomposition rate of ozone:

$$-\left(\frac{d[O_3]}{dt}\right)_{total} = 2k_3[O_3][O]_{ss} \tag{13}$$

Combining equations (8) and (13), which describe ozone's decomposition dependence on O_2 concentration, yields:

$$-\left(\frac{d[O_3]}{dt}\right)_{total} = 2k_3[O_3]k_1[O_3][M]/k_2[O_2][M] + k_3[O_3] \tag{14}$$

Two special cases at standard temperature pressure (STP) will be examined:

Case A. High ozone concentration limit where $[O_3] \gg [M]$ and $[O_2] = [M]$. Taking a typical O_3 concentration of 98% and a 2% O_2 yields:

$$-\left(\frac{d[O_3]}{dt}\right) = (9.29)10^{-9} \text{ mole}/(\text{liter} \times \text{sec})$$

Thus the percent decomposition rate of O_3 would be $R_1 = (2)10^{-5}$ in percent per sec.

Case B. Low ozone concentration limit where $[O_3] \ll [M]$. Assuming a 5% ozone concentration and 95% oxygen, the ozone percent decomposition rate would be: $R_2 = (1.6)10^{-7}$ in percent per sec.

Comparison of R_1 with R_2 shows that the percent decomposition rate of O_3 at high ozone concentration is about 125 times faster than the percent decomposition rate of O_3 at low ozone concentration. Therefore the initial presence of O_2 is a major factor determining the ozone decomposition. Not only oxygen, but small amounts of hydrocarbonic impurities (such as H_2 and Br_2) found in the vacuum system are efficient catalysts and can sensitize rapid ozone decomposition leading to explosions. In addition, many solid substances such as coal and metal (Fe, Pt group)--especially silver--are very active catalysts (ref. 23). It is therefore important to recognize that decomposition of ozone depends on the particular strongly vacuum system that has been used.

Pure ozone is photochemically decomposed when exposed to visible or UV light. Visible light is proposed to decompose O_3 into O_2, the mechanism being $O_3 + h\nu \longrightarrow O_2 + O(^3P)$. The O atom (at the ground state ^3P) will react with another ozone molecule, $O + O_3 \longrightarrow O_2 + O_2$. Thus, in spectroscopic studies of ozone's thermal decomposition, unnecessary exposure to light should be minimized.

Safety and Precaution

Ozone is second to flourine in its oxidation potential. This means that ozone will react with most materials, which will lead to the destruction of ozone and impurities from the oxidized materials. Therefore, only glass and teflon could be used in the apparatus because they are resistant to oxidation and ensure the cleanliness of the system; this limited the quantities of impurities that could affect the ozone concentration. The use of these inert materials was also important for safety because the decomposition can be very rapid when there is a high concentration of ozone, resulting in explosions. Care was taken to limit the impurities, minimize vibrations, and ensure that there would be no sudden pressure or temperature variations--all of which could lead to the rapid decomposition of ozone. In addition, the use of silica gel was helpful because it safely stores quantities of ozone. Also, nonhydrocarbon vacuum pump oil was used because it does not react with oxygen and ozone as regular hydrocarbon oils do. As an added precaution, goggles and face shields were used and a shield of plexiglass was erected in front of the apparatus to protect the operator from flying glass caused by an explosion. Inhalation of ozone should be avoided; a threshold limit value of 0.1 ppm of ozone in the air has been established by the American Conference of Government Industrial Hygienists. For this reason an exhaust fan was installed in the lab.

EXPERIMENTAL APPARATUS

Experimental Setup

The experimental apparatus included an ozonizer pump for initial evacuation and purification of ozone, pressure gauges, cell and coolant

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system, and spectrophotometer with recording system. A diagram of an ozone generating system is shown in Figure 4. All valves are teflon or stainless steel. The glass trap containing silica gel was joined to the stainless steel portion of the system using a kovar seal. In Figure 4 the high vacuum portion of the system, which was stainless steel, is represented by thick solid lines; the teflon valves, 0.63 cm inside diameter, are marked by

⌐T#⌐   ; and the stainless steel valves are designated by   ⌐S#⌐   .

Ozonizer

The ozonizer is a sealed box which contains six glass tubes 65 cm in length and 5 cm in diameter. The glass tubes cover stainless steel foils which are connected in a series to serve as an electrode (Figure 5). The production of ozone was initiated by the introduction of O_2 into the ozonizer which generated ozone by the silent electrical discharge method. This method is considered to be the most practical way to quickly produce a large quantity of ozone for laboratory purposes. This electrode was connected to a potential difference capable of generating 15 kv-AC while passing a current of about 3 amps. The operation of the ozonizer required a steady current of water to keep it cool. Under these conditions the ozonizer generated about 2% ozone for an oxygen flow of 4 liters per minute. For an experimental run the ozonizer was operated anywhere from 15 to 30 minutes while the generated ozone was trapped in the silica gel.

Pumps

Three different types of pumps were used to prepare the system and to purify the created ozone.

1. A mechanical roughing pump contained silicon base oil in order to minimize interaction with ozone. The pump was connected to the system with a Linde molecular sieve type 13X which is a good catalyst to decompose ozone, thus limiting any ozone getting into the roughing pump. This pump provided a vacuum as low as 50 microns during the cleanup of the ozonizer. After the silica gel was saturated by gaseous ozone the pump was used to remove residual oxygen and other impurities.

2. A Varian vac-sorb roughing pump operating at 70 microns to 10^{-4} torr and containing absorbent material was employed to provide the base pressure for starting the vac-ion pump. This pump was not used during the purification process.

3. A Varian vac-ion pump of 20 liters per second was initially used to obtain a high vacuum in the cell and then to pump on the liquid ozone. The operating pressure range is 10^{-3} to 10^{-7} torr for a non-baked system.

Pressure Gauges

The cell pressure was measured by a 222HS-A-1000 series of MKS Baratron electronic manometer. This is a stainless steel manometer which operates on the variable capacitance principle with response time of 5 msec and an accuracy of 1.5%. The input voltages are ±15 DC which are maintained by two independent power supplies. The output is displayed on a digital voltmeter. The Baratron measurements were calibrated before the experiment against a mercury manometer at room temperature, noting that no compensation for temperature is needed in the operating range from 0° to 100° C. Pressures during purification and evacuation of the system between 1000 and 10 microns were read on a Hasting vacuum gauge type DV-6M and lower pressures were measured using the vac-ion pump.

The Absorption Cell

The absorption cell (Figure 6) has a triple quartz wall with double supersill windows. The cell was used to confine a purified sample of gaseous ozone through a teflon valve and then to study the dependence of absorption coefficients on temperature. Low temperatures were achieved by passing cooled, vaporized N_2 through the space between the inner and middle walls. A stable temperature for the gas sample was achieved by wrapping the cell and the teflon valve with 10 layers of glass wood-insulating material. This temperature was measured with a type K (chromel-alumel) thermocouple with reference junction at 0° C, inserted between the inner and middle walls of this cell. This temperature was monitored on a digital electrometer (Keithle 616 electrometer). Condensation of water vapor on the windows of

the cell was avoided by the evacuation of the space between the middle and outermost walls. In addition, thermal exchange was minimized by coating the outside surface of the outermost cell with silver. The following are the detailed specifications of the cell.

1. Innermost cell: 8 cm in length, 2 cm in diameter with an inlet from outside (5 cm) which had an 0.37-cm inside diameter; the windows were glass-to-glass sealed.

2. Inner cell: enclosed with a glass cover and sealed off before the windows, thus designating the middle cell.

3. Outermost cell: total length, 13 cm; diameter, 38 mm, concentric with the inner cell having glass-to-glass sealed windows.

4. Space between middle and outermost walls was initially evacuated to 10^{-6} torr.

5. Space between innermost and middle walls was accessible by two glass tubes 0.635 cm in diameter for passing coolant to obtain temperature control.

6. Distance between innermost and middle walls was 4 mm.

Cooling Technique

Temperature was controlled by forcing N_2 from a pressurized tank, which was passed through liquid nitrogen, into a 50-liter stainless steel dewar. The inlet tube was made of copper and was immersed in liquid nitrogen. Passing of N_2 through the copper tube caused the liquid to vaporize, creating a positive pressure inside the dewar. An insulated teflon tube above the liquid level then transported the cold nitrogen vapor around the cell. By adjusting the rate of the flowing N_2 into the dewar the required temperature was obtained. With this technique temperatures as low as -150° C were produced. The time required to reach such a temperature was five to ten minutes depending on the flow rate of N_2 into the container and the level of liquid nitrogen in the dewar. In order to raise the

temperature, the outlet of the dewar from the cell had to be disconnected and the inlet side of the cell had to be attached directly to the dry N_2 valve of the laboratory by means of another copper tube. Then, by heating the copper tube, temperatures up to 80° C could be obtained (Figure 7).

Spectrophotometer

The absorption coefficients were measured by a Perkin-Elmer Model 200 dual-beam spectrophotometer with a variable spectral band pass from 0.2 to 4.0 nm. The accuracy of the band pass was confirmed by using iodine gas. In this experiment the band pass was set to 0.3 nm so that high resolution was sufficient throughout. The light sources were a tungsten lamp for the visible and a D2 source for the UV. These light sources together with the electronics require a warm-up time of approximately 45 minutes to achieve stable operation. To maintain long-time variation a calibration was done before each experiment by taking the absorption spectrum of the empty cell for the required spectral range.

The spectrophotometer is designed to compare the light intensity passing through the sample with the light intensity passing through the reference cell (Figure 8). Because of the space requirement for the sample cell insulation, the reference cell was removed, leaving a space in the optical path instead of the reference cell. The absorption coefficient, which is constant throughout the gas, can be calculated from Beer's Law:

$$I = I_o e^{-\alpha x} \tag{15}$$

where I_o is the intensity of the light entering the gas and I is the intensity exiting the gas cell with the thickness x. To correct for the cell windows' absorptions, the absorption of the empty cell was recorded. Thus:

$$I(\lambda)_{empty} = I_o A_{cell}(\lambda) \tag{16}$$

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And for the gas-filled cell:

$$I(\lambda)_{gas} = I_o(\lambda)A_{cell}(\lambda)e^{-\alpha x} \qquad (17)$$

Dividing equation (17) by equation (16) we obtain:

$$\frac{I_{gas}(\lambda)}{I_{empty}(\lambda)} = e^{-\alpha x} \qquad (18)$$

Solving for α we obtain:

$$\alpha = \frac{1}{x} \log \frac{I_{gas}}{I_{empty}} \qquad (19)$$

Then the absorption coefficient at standard temperature and pressure would be $\alpha_{stp} = \frac{(76)T}{273P} \alpha$ (temperature is in degrees kelvin and the pressure is in cm of Hg).

Analog-To-Digital Converter

The output signal from the spectrometer takes on values from 0 to 1 volt, which corresponds to 0% and 100% of absorption. These signals were fed directly into the North-Star Horizon microcomputer. The signals had to be first amplified by a factor of 10, then converted by an ANALOG-TO-DIGITAL MODULE that interpreted the 0- to 10-volt signal to an integer data from 0 to 1023; the accuracy of determining the percent absorption was then 100/1023.

XY Recorder

The variation of the absorption with temperature for a fixed wavelength was monitored on the Y-axis and X-axis of a Gould Brush 500 XY recorder. The X-axis input was connected to the spectrometer and the Y-axis to the thermocouple. The recorder was calibrated to known voltages (voltage calibrator, DCV 8500) prior to the experiment.

EXPERIMENTAL PROCEDURE

The experimental procedure is divided into four parts: purification and pacification of the system; creation of ozonized oxygen, purification of ozone; and measurement of absorption coefficients of ozone in the absorption cell. Descriptions of each part follow.

Part I. The complete system with the exception of the ozonizer and silica gel cold trap was helium-leak tested; then, using the roughing pump, the complete system was evacuated. The silica gel, used to absorb small quantities of ozone safely, can easily absorb moisture which was removed by baking the silica gel while pumping with the vac-sorb pump. This procedure made it possible to attain a pressure as low as 8 microns. In the next step the glass, teflon valve and fittings of the vacuum system, and the MKS baraton were exposed to ozonized oxygen for two days in order to pacify the system. This is a normal procedure used to reduce the impurities during the process of making ozone. Once the system was pacified, all valves except the venting valve (#2) and oxygen inlet valve (#1) were opened. Then a roughing pump was used to obtain a vacuum down to 50 microns. A high vacuum was then obtained in the cell, isolating it from the rest of the system by closing valves #12 (pumping main valve), #6 (valve separating the final cold trap from double trap), and #5 (pressure gauge valve). At this point the vac-sorb pump was cooled with LN_2 to reduce the pressure so that the vac-ion pump could be started. Once the pressure was reduced to 10 μ the system was isolated from the vac-sorb pump by closing valve #13 (vac-sorb valve). Thus evacuation of the cell continued until 10^{-6} torr was reached. While the vac-ion pump was working on the cell, ozone was created.

Part II. The dewar under the silica gel cold trap was filled with a mixture containing dry ice and alcohol. This produced a stable temperature of -78° C in the silica gel. The water circulated around the ozonizer was turned on to remove the dissipated energy from the ozonizer. This was accomplished by a constant current of water (about 14 gal/hour). The next step in the procedure was to close valve #14 (roughing valve) and to fill the system with pure oxygen. This was accomplished by opening valve #1 (inlet oxygen valve) and monitoring the pressure until a slight over-pres-

sure was detected. Then valve #2 (venting valve) was opened and oxygen was allowed to pass through the system to remove the trapped impurities. This was necessary to allow the electric discharge to occur in pure oxygen. Then the ozonizer was turned on with a 75-volt reading on the input transformer-- noting a current of 3 amps. This procedure produced ozonized oxygen with 2% ozone concentration. The positive oxygen pressure forced the ozonized oxygen to pass over a bed of silica gel that selectively absorbed the ozone, allowing the oxygen to pass out of the system. After 10 minutes the silica gel turned blue and the ozonizer was turned off, followed by the closure of valves #2 (venting valve) and #1 (inlet oxygen valve). At this point the created ozone in the silica gel was isolated from the ozonizer by closing valve #3 (inlet ozonized oxygen valve).

Part III. Ozone was purified by the following steps: (1) Valve #14 (roughing valve) was opened slowly which allowed the remaining oxygen in the silica gel cold trap to be pumped out. After pumping on the silica gel for 45 minutes, the pressure reduced to 120 microns. At this point pumping had to be stopped to remove ozone. (2) The ozone was further purified when passed through the double trap to the single cold trap. In order to do so the dewar under the double trap was filled with dry ice and alcohol while valves #11 and #7 were closed (valve #11 connects the glass section to the stainless steel portion and valve #7 connects the single trap to the teflon tube). In the next step, valves #6 and #5 were opened (valve #6 separates the final cold trap from the double trap and valve #5, between the cold trap and the MKS pressure gauge). Subsequently the dewar of liquid nitrogen (77 K) was put under the single trap. The process of transferring ozone into the single cold trap was started by increasing the temperature of the silica gel. Thus, only impurities that do not freeze below -78° C were allowed to pass through the double cold trap, while the ozone accumulated in the single cold trap. (3) Purification of liquid ozone proceeded by closing valve #6. Thus the pump was allowed to operate on the cold trap until a pressure of 50 microns was reached. Since the vapor pressure of oxygen is about 130 mm Hg at LN_2 temperature and the vapor pressure of ozone is only about 0.1 mm Hg, the pump was used to remove oxygen from the trap, leaving the ozone. (4)

Further purification was performed after the ozone was distilled into the double trap. In order to do so, first the double cold trap had to be cleaned by increasing its temperature and evacuating it (valve #11 was opened until a pressure of 50 microns was obtained). Subsequently, valves #5 and #10 (separating silica gel from the double cold trap) were closed and LN_2 was placed under double cold trap. In order to transfer the ozone from the single trap to the double trap, valve #6 (located between the single and double cold trap) was opened and the single cold trap was heated. At this point pumping on the double trap was initiated by opening valve #5 (pressure gauge valve). The pressure was again reduced to about 50 microns. Valve #6 was closed and liquid ozone was vaporized by removing the LN_2 dewar. This provided a fairly purified gaseous ozone. To further absorb impurities that freeze below -78° C, the double cold trap was enclosed by a mixture of dry ice and alcohol. Thus the gaseous ozone in the double cold trap served as a reservoir for the remainder of the experiment. (5) Small amounts of ozone were transferred into the single cold trap for final purification. This was done by closing valve #5 and opening valve #6 for a short period of time. Then LN_2 was placed under the single cold trap and valve #7 was slowly opened so that pumping by vac-ion pump could proceed until a pressure of 10^{-6} torr was achieved. (6) To free any trapped impure molecules mixed with liquid ozone, valve #7 was closed allowing the liquid ozone to slowly vaporize by removing the LN_2 under the trap. This process allowed the adhered impurities together with the ozone to be brought into gaseous state. At this point the LN_2 was re-introduced under the trap, liquifying the ozone while releasing some of the adhered impurities. These residual impurities were removed by opening valve #7 and pumping until a pressure of 10^{-6} torr was reached. The fact that oxygen at LN_2 temperature has a vapor pressure of 130 mm of Hg indicates that at a pressure of 10^{-6} torr the liquid should be 100% pure ozone. It is worth noting that the vaporization of this liquid, which took 10 minutes, was not accompanied by decomposition. (This is discussed later in this report.) The gas that was produced was used to fill the cell for measuring the temperature dependence of the absorption coefficients.

Part IV. The followings steps were taken to measure the absorption coefficients: (1) During the 10 minutes when the vaporization of ozone in

the single cold trap occurred, the reference spectrum of the evacuated empty
cell was recorded. The spectral region between 7567 Å and 4630 Å was
scanned, taking about 10 minutes. This produced a spectrum which was used
for background correction. (2) The next step was to fill the cell with
ozone which was isolated from the vac-ion pump by closing valve #7. To
measure the pressure in the cell, valve #4 was closed and valve #5 was
opened long enough to read the pressure. This avoided any decomposition of
ozone on the surface of the stainless steel in the MKS pressure gauge. Then
valve #9 (valve to the cell) was closed until the end of the experiment.
(3) Several scans were taken with the filled cell in the optical path of the
spectrophotometer. At the end of each scan the wavelength was automatically
set to the same starting point. The low temperature spectrum was obtained
by cooling the cell for approximately 20 minutes--enough time for the con-
fined molecules to reach equilibrium. To raise the temperature, dry N_2 gas
was circulated around the cell, requiring about 20 minutes to stabilize. In
addition to the above procedure for measuring, the variation of absorption
coefficients on temperature was monitored by selecting a fixed wavelength
while changing the temperature. These results were recorded on an XY
recorder.

RESULTS AND CONCLUSION

Several sets of absorption coefficients in the visible region were
obtained by changing the temperature of the purified confined gas sample.
These measurements were performed using a spectrophotometer with an 8-cm
quartz absorption cell. The technique for determining temperature depen-
dence was different from those used by previous investigators (for example,
photoelectric detectors, pure ozone, and a capacitance pressure gauge were
used instead of photographic detectors, ozonized oxygen, and a sulfuric acid
manometer). The absorptions recorded at room temperature in the visible
region can be compared with those previously reported.

The absorption spectrum obtained in this work together with those of
Inn's and Tanaka's, Vigroux's and Griggs' are shown in Figure 9. The gen-
eral spectral features found in the present work agree closely with Inn and

Tanaka except that in the present work the difference in absorption coefficients between the two peaks was the same as that reported by Vigroux; Inn and Tanaka reported a smaller difference. Our measurements could differ from Inn's and Tanaka's because their values for the absorption coefficients were reached using interpolated decomposition values. They reported 10 to 12% thermal decomposition of O_3 over a period of 5 to 10 minutes. On the other hand we vaporized and liquified our ozone ten times in the sealed cold trap during a period of 90 minutes, showing only 0.3% decomposition.

The temperature effect was examined in this study by measuring the absorption coefficients for the Chappuis band in a sealed-off, gas-filled cell raised to different temperatures. The study consisted of three runs. In the first two runs there were several continuous spectral scans at different temperatures; in the third run, variations of absorption were recorded for specific wavelengths as a function of temperature. In each run the evacuated cell (10^{-6} torr) was filled with pure ozone at room temperature. The pressures for the first, second, and third runs were 24, 37, and 45 cm Hg respectively.

During the first run three scans were taken, each scan starting at 4630 Å and stopping at 7567 Å. The first scan was obtained at room temperature of 303 K and pressure of 24 cm Hg. The absorption coefficients are exhibited in Figure 10. The second scan was performed thirty minutes later at a temperature of -108° C (thirty minutes were needed to cool the cell from room temperature). Having completed the second scan, the cell was brought back to room temperature and the third scan was obtained about 30 minutes later. The absorption coefficients of the second and third scans are shown in Figures 11 and 12 respectively. Using computer program ozone (Appendix B), the difference between the first and the last scan is illustrated in Figure 13, showing a shift of 0.0008 cm^{-1} (base 10) in the background. Figures 14 and 15 show the differences between the first and the last two scans. These figures signify an overall increase in absorption coefficients with a maximum of 6% at $\lambda = 6020$ Å in going from room temperature to -108° C. In addition to the overall increase of absorption coefficients, there seemed to be local maximums and minimums (Figure 15)—between 6000 Å and 4630 Å—but because the wavelength reproducibility was 10 Å we were unable to determine the wavelength associated with these various regions.

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In the second run which lasted 44 hours, seven scans (Figures 16-22) of absorption coefficients were performed starting at 4630 Å and stopping at 7567 Å. The first four of these spectrums were taken successively, each 25 minutes from the previous one. In order to evaluate the quantitative decomposition of ozone in the absorption cell, the last two scans were performed 43 and 44 hours after filling the cell (Figures 21 and 22). The fill temperature and pressure of the ozone in the absorption cell for the second run was 303 K and 37 cm Hg. Using the fill condition, a spectral scan was performed (Figure 16). The next scan was performed at 198 K, noting that the maximum increase (4.5%) occurred at $\lambda = 6020$ Å (Figure 17). The third scan was obtained at 30° C (Figure 18). We reproduced the conditions of scans 2 and 3 for scans 4 and 5 except that the low temperature for the fourth scan (Figure 19) was -108° C. The fifth scan (Figure 20) was taken 1.5 hours after the fourth one. At this point we examined the difference between low- and high-temperature spectra. The differences between the first and second scans and the third and second scans are exhibited in Figures 23 and 24. The difference between the third and fourth scans is associated with the largest temperature differential, and showed a 6% increase at $\lambda = 6020$ Å (Figure 25). The difference of absorptions between scans 3, 5, and 7 from the first scan are shown in Figures 26, 27, and 28 respectively. These figures, in particular Figure 28, were used to evaluate the decomposition rate which was found to be approximately 0.3% per hour.

The fill pressure in the third run was 45 cm Hg at room temperature. Selecting wavelengths on the spectrophotometer, we monitored on an XY recorder the absorption while the ozone was liquified (at T = -111.9° C) and then vaporized and finally brought to room temperature. Each process of cooling and heating took 15-20 minutes. In Figure 29 the Y axis represents the absorption of 0% to 100% and the X axis represents the temperature in C. On each graph cooling and heating is designated by C or D respectively. Analyzing these graphs reveals that for the fixed wavelength chosen at several peaks and valleys the variation of absorption coefficients as a function of temperature is linear (shown in Table 2).

Table 2. Slopes of the variations of absorption coefficients as a function of temperature for fixed wavelengths.

Wavelength (Å)	5200	5698	5858	6020	6500
Slope $(mV.c^{-1}).10$	5	8	7	11	4

It is worth to mention that there was a temperature difference between the cell and its inlet tube, introducing some errors. Examining this effect the calculations were carried out with the result that a 100° C temperature difference would introduce only 0.8% in ozone absorption.

The spectrums in the first two runs lead to the firm conclusion that this band is temperature dependent with maximum change in absorption of 5% at $\lambda = 6020$ Å for a difference temperature of -108° C to 30° C, whereas the reported values were 1% to 2%.

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(a) GVB CONFIGURATIONS OF O_2

A   x   B

z
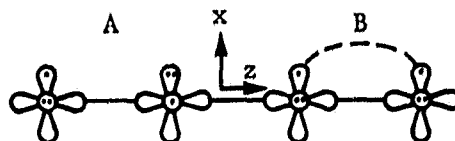
(b) GVB CONFIGURATIONS OF O_3

π^4 π^5

GOOD   BAD
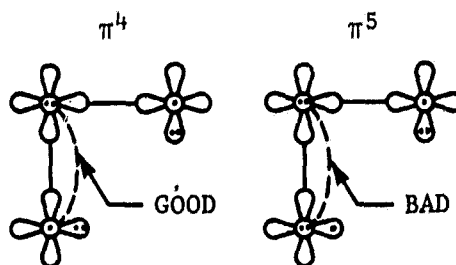
(c) THE π^4 CONFIGURATION OF O_3

ϕ_c ϕ_r

ψ_ℓ

PAIR–PAIR
REPULSION
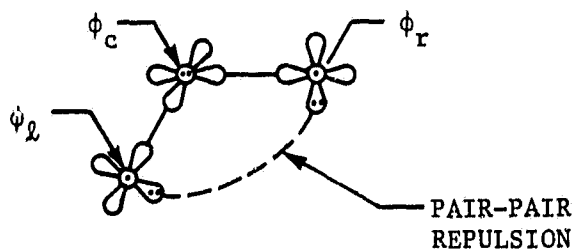
Figure 1. A schematic representation of the GVB orbitals.
The P orbitals are represented by a normal two-
lobed shape, if in the plane and a circle if
perpendicular to the plane. (a) The bonding
GVB configurations O_2. The bonding GVB con-
figurations of O_3. The upper two O atoms,
represent the original O_2 molecule to which
the lower O atom is added, resulting in the
two configurations shown. (c) The π^4 configu-
ration of ozone.

26
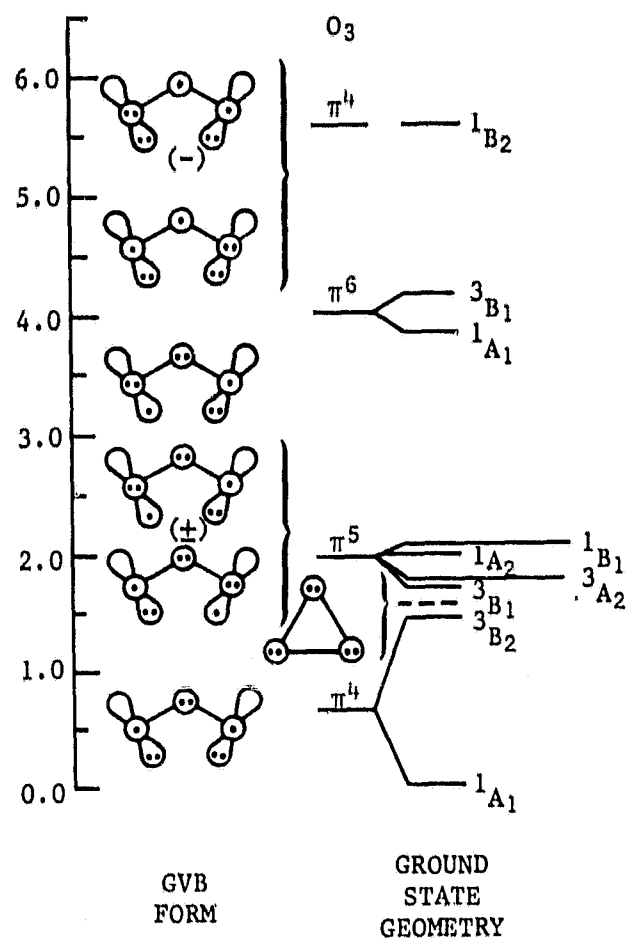
Figure 2. The energy levels of O_3 shown based upon the theoretical calculations.

O_3 (R = 2.415)
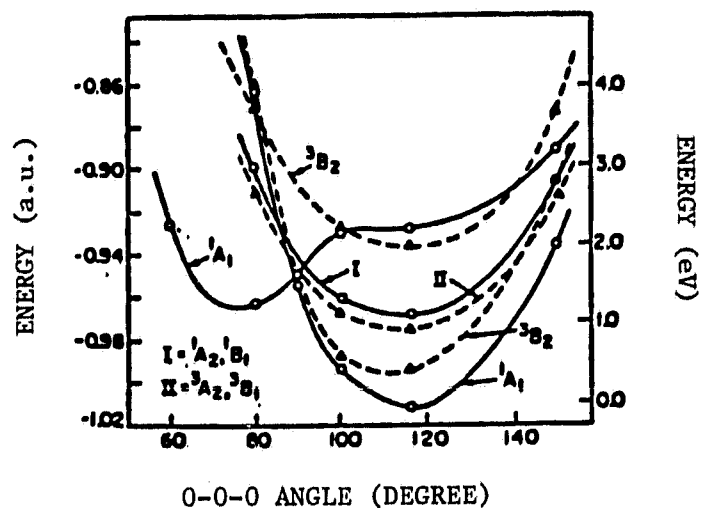
Figure 3. The energy curves (GVB) for the excited states of ozone. In these calculations the O-O bond length was kept fixed and only the angle varied.
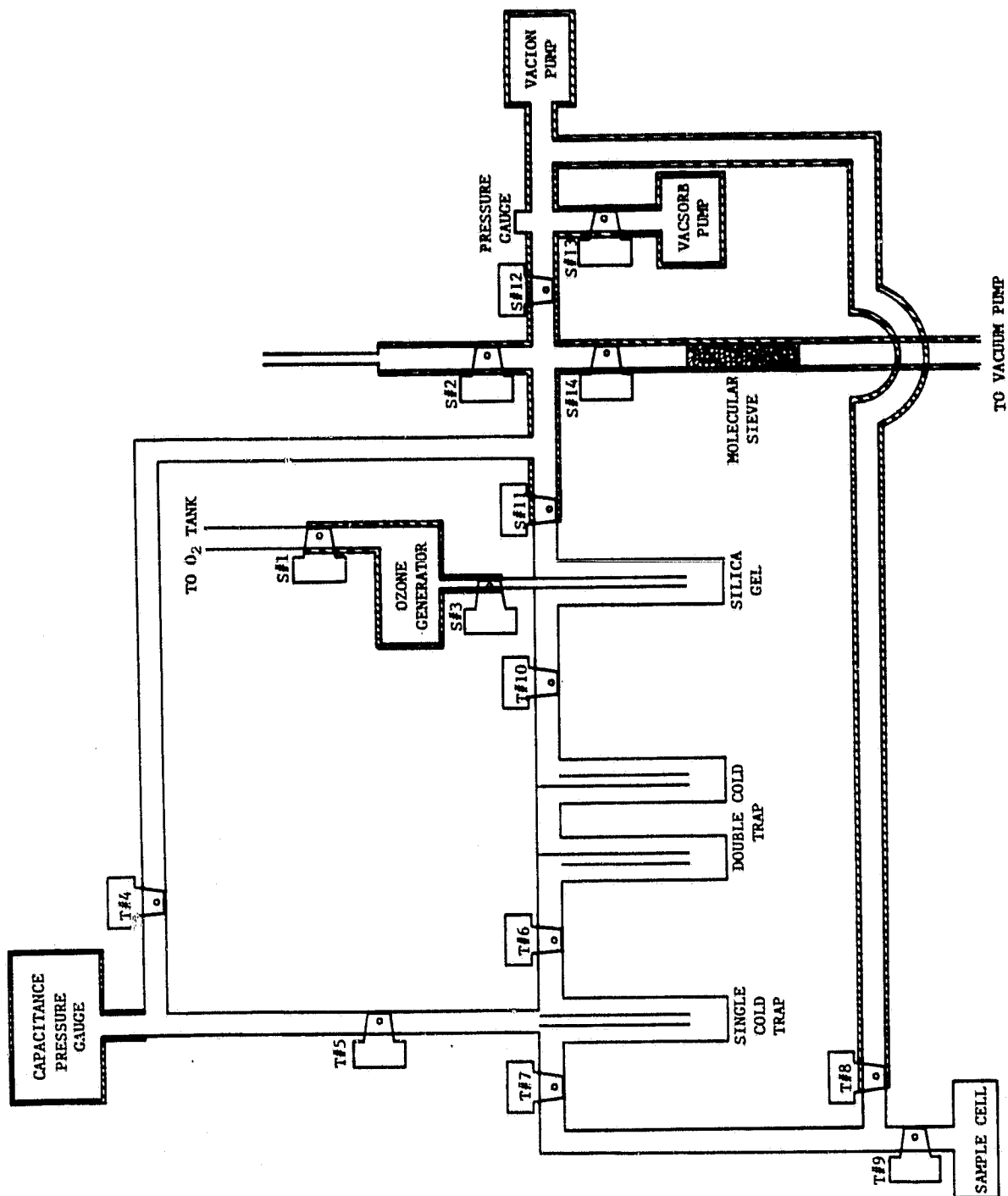
Figure 4. Diagram of ozone generating system.
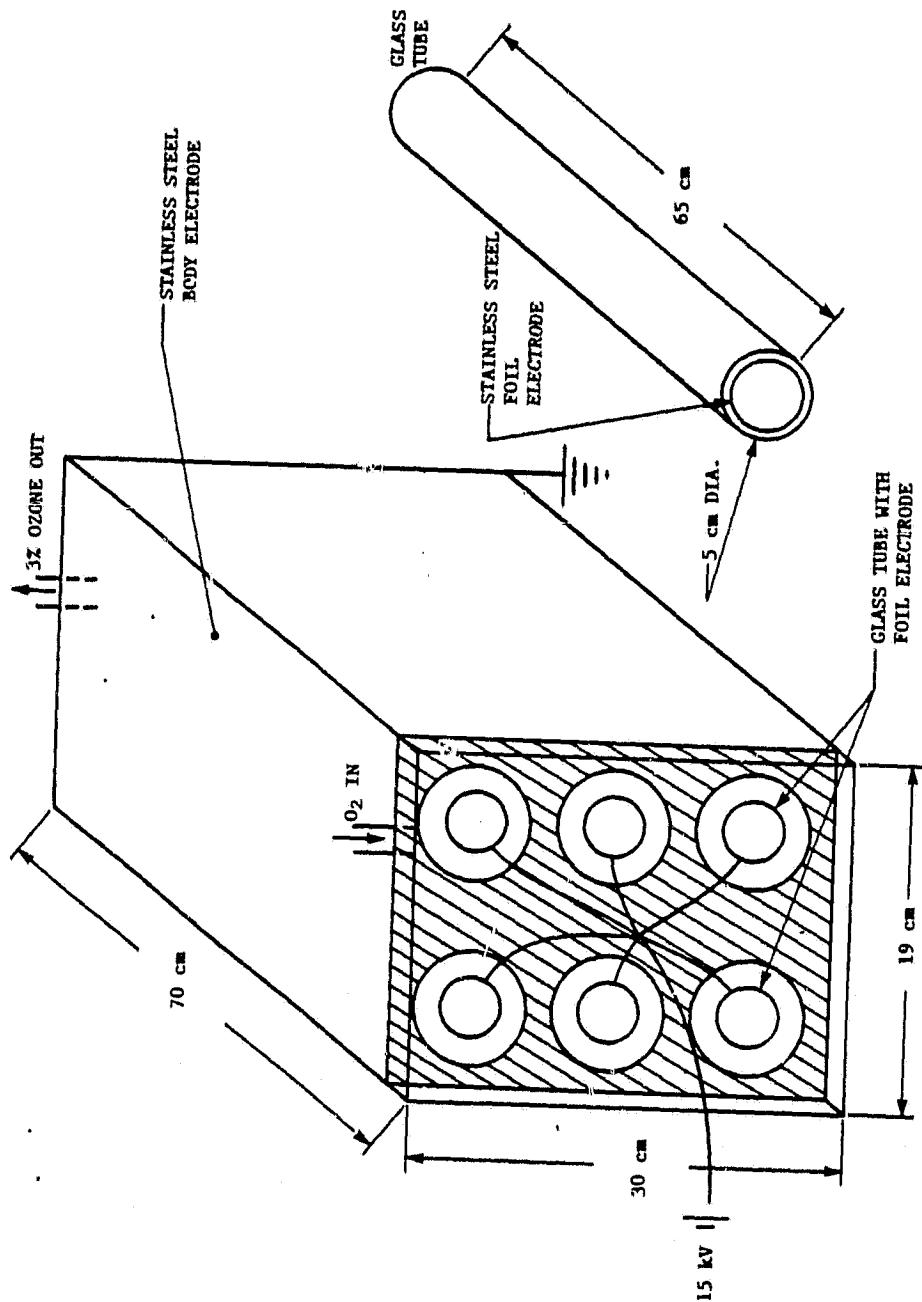
Figure 5. Schematic diagram of ozone generator.
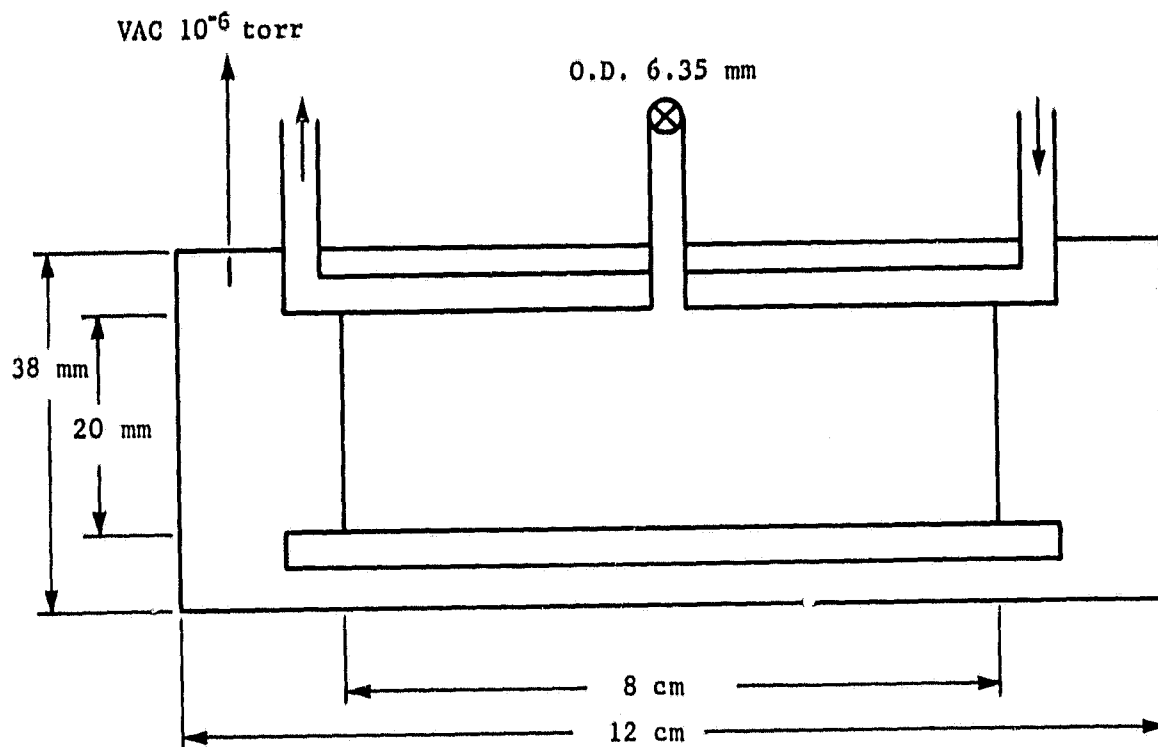
Figure 6.   Schematic of the absorbtion cell.
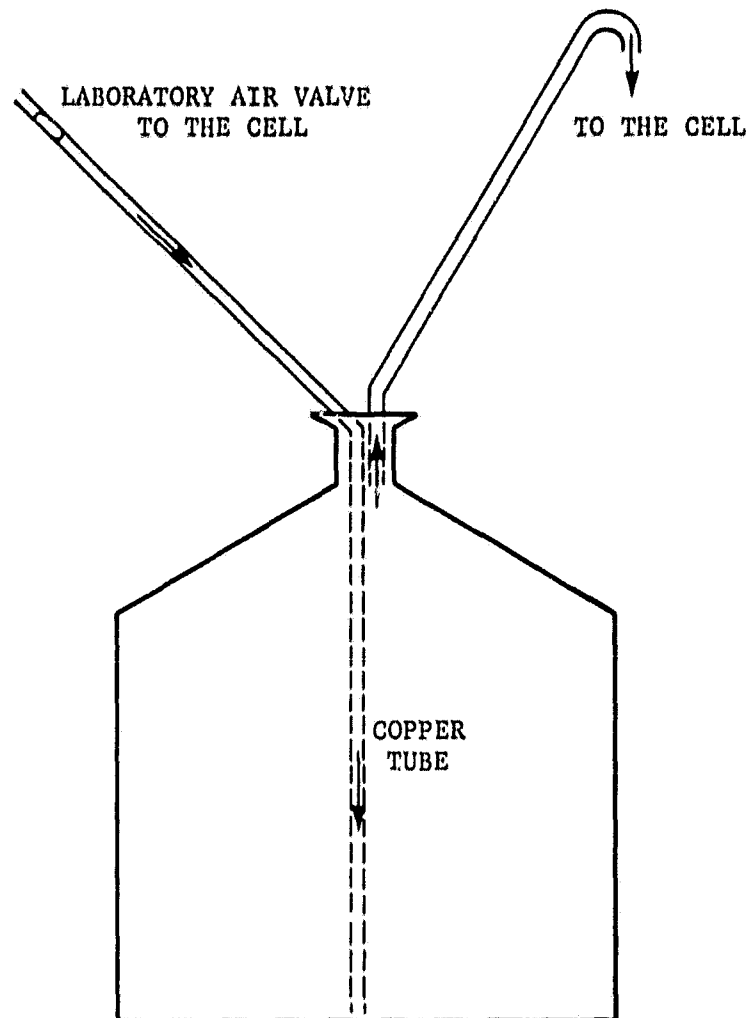
Figure 7. Schematic of the stainless steel container.
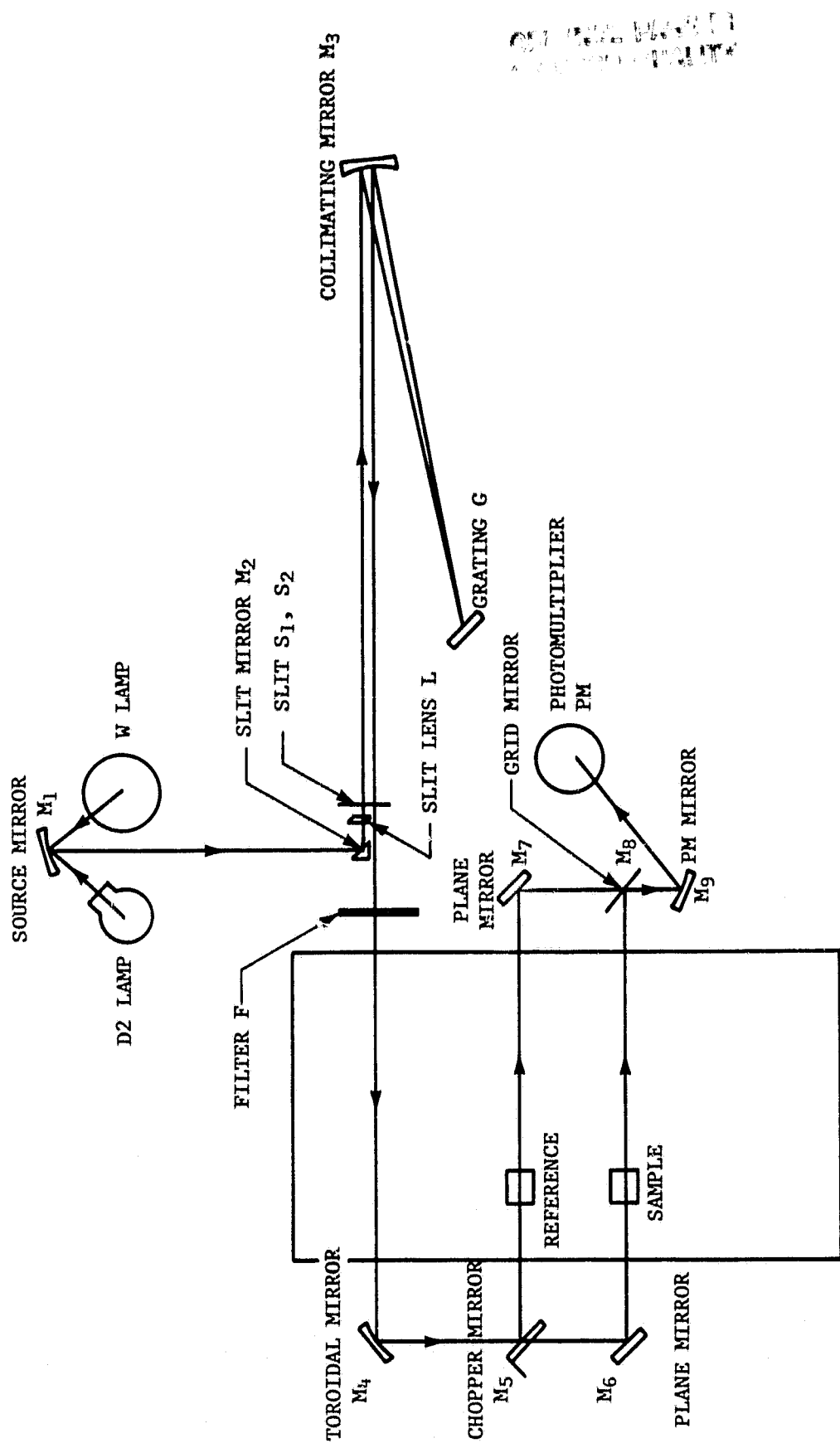
Figure 8. Optical schematic, Model 200 Spectrophotometer.
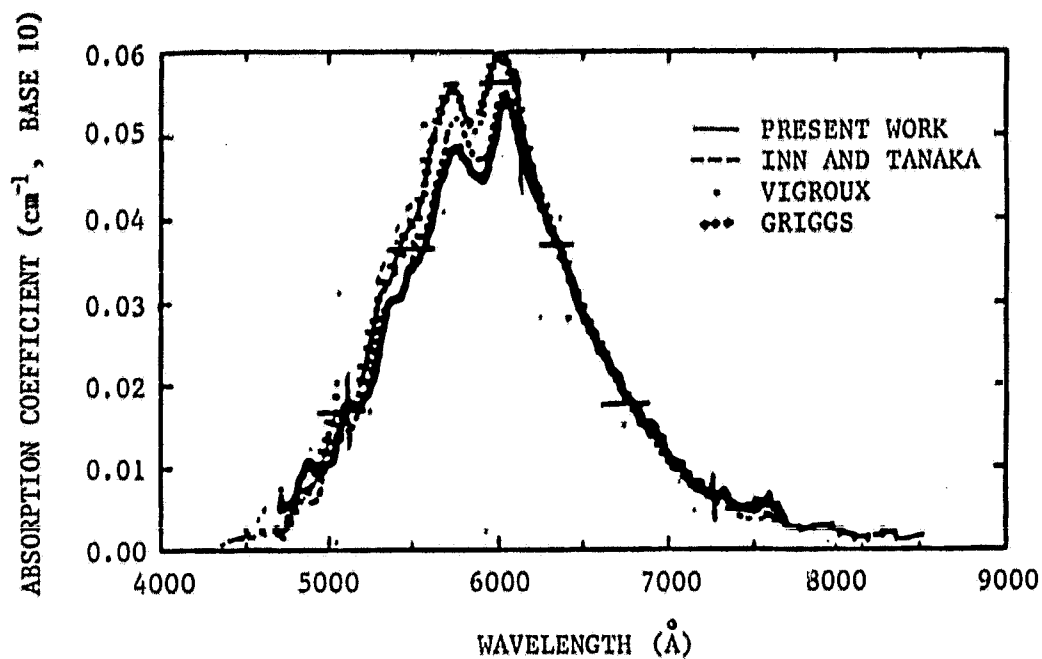
Figure 9. Chappuis band (4400-8500 Å) absorption coefficients.
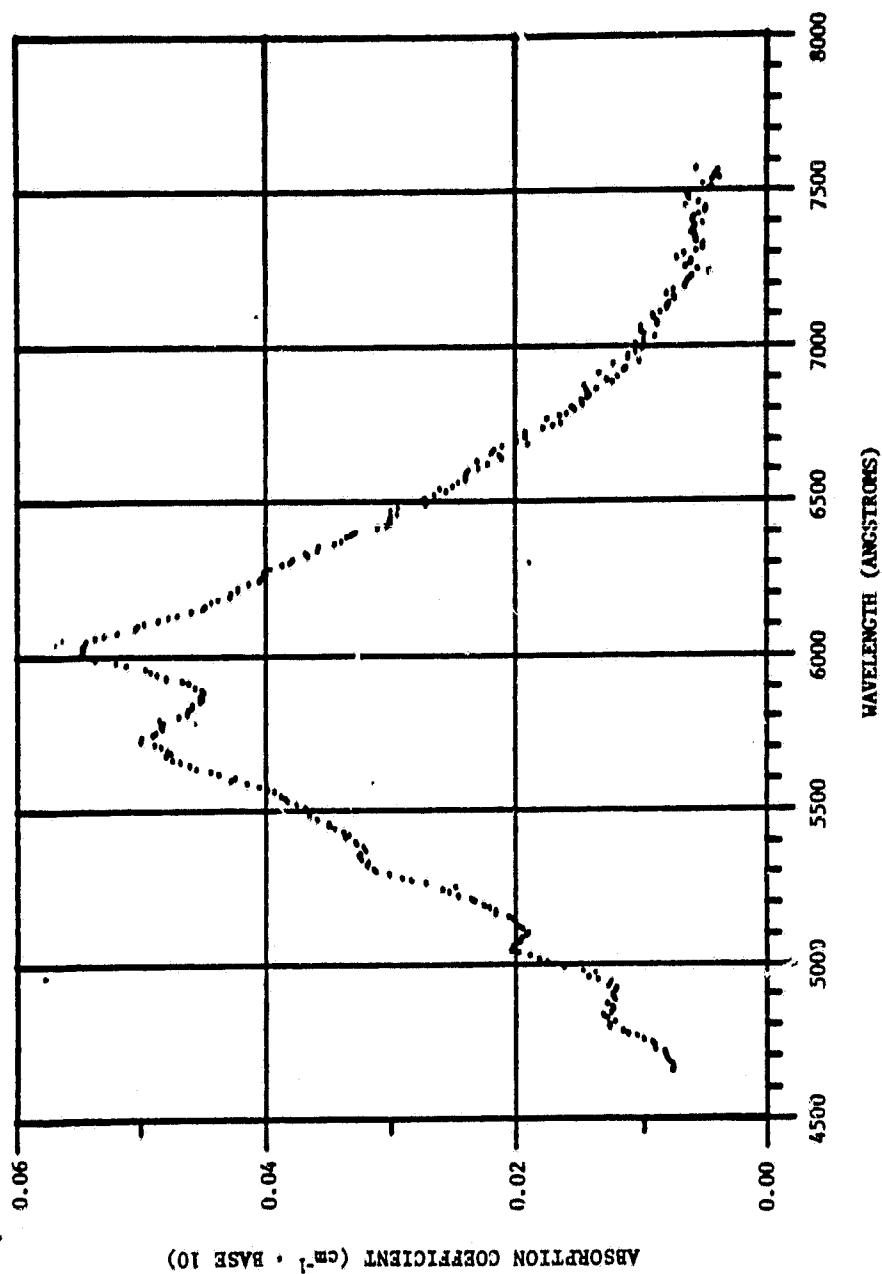
Figure 10. Calculated absorption coefficients of ozone at STP, using a gas sample at T = 303 K and P = 24 cm Hg (fill 1).

35
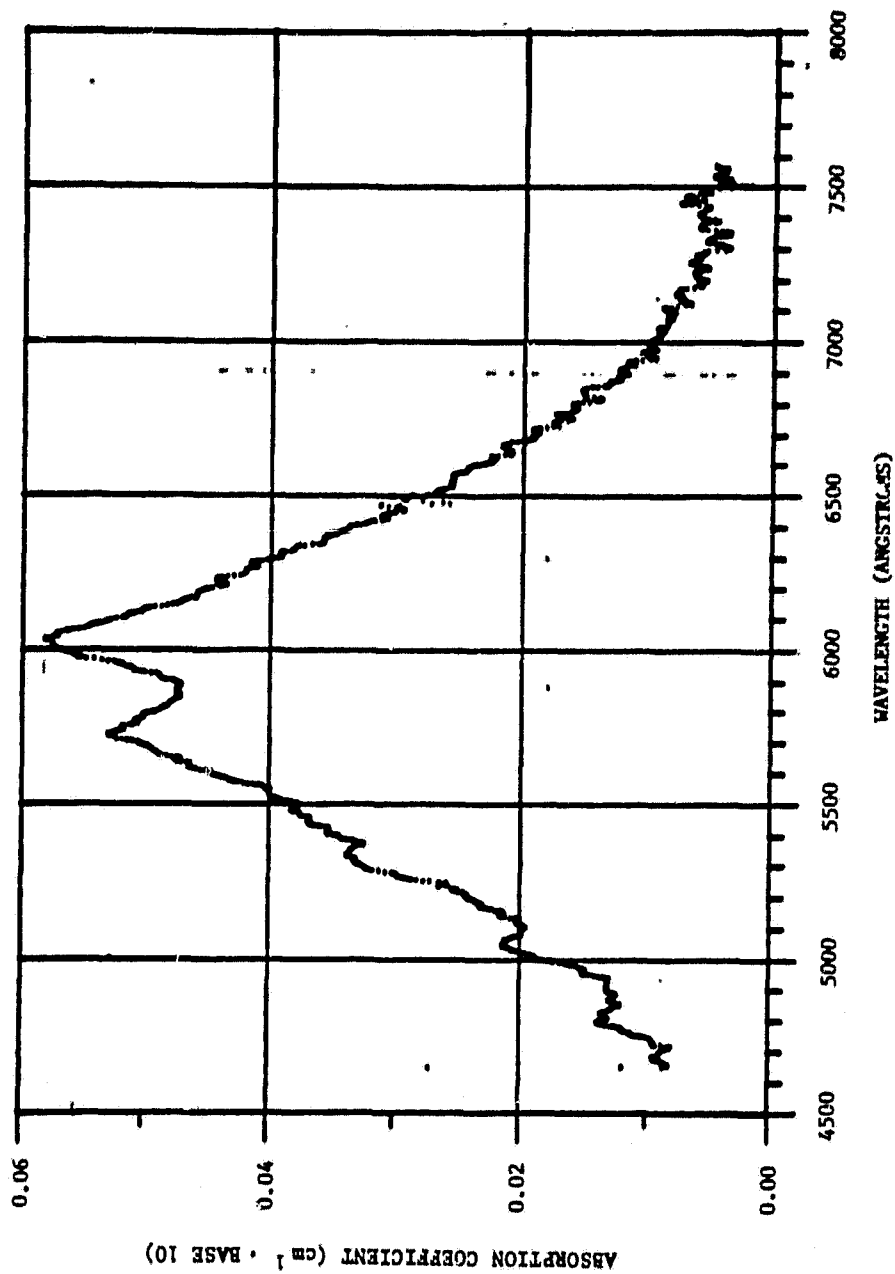
Figure 11. Calculated absorption coefficients of ozone at STP when temperature of the gas was decreased from 303 K to 165 K (50 minutes after filling) at P = 24 cm Hg (fill 1).
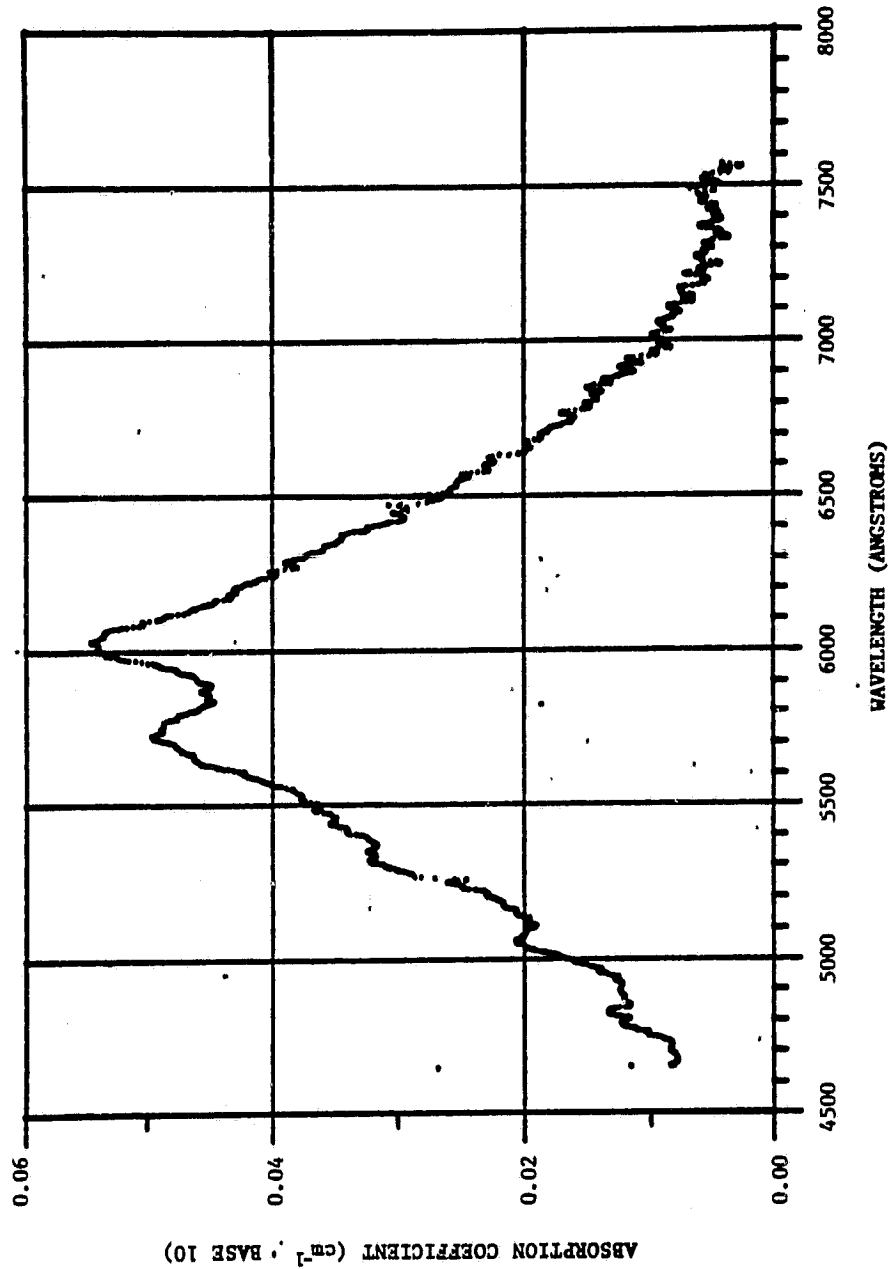
Figure 12. Calculated absorption coefficients of ozone at STP (90 minutes after filling) at T = 303 K (fill 1).
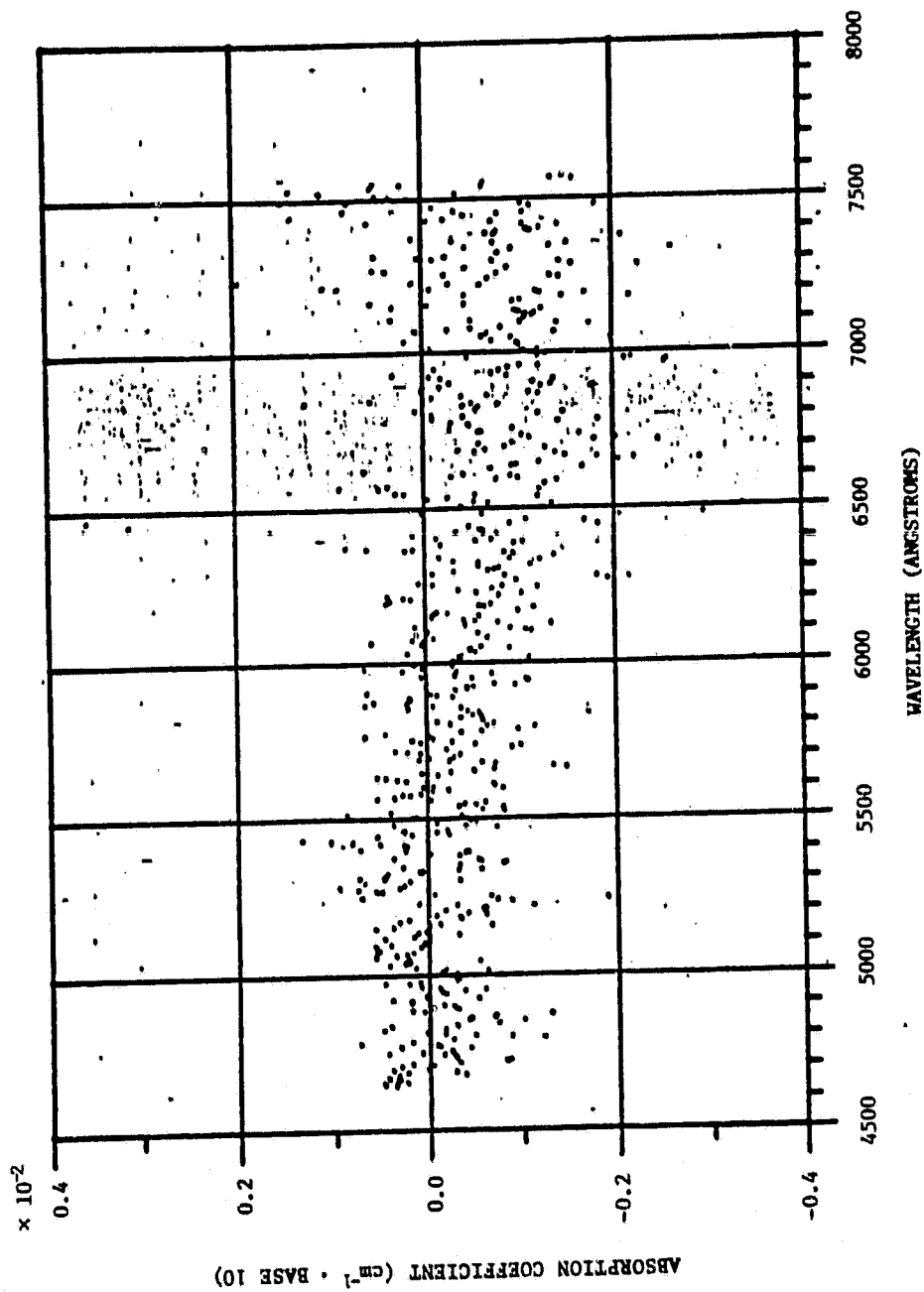
Figure 13. Difference of absorption spectrum at T = 303 K (time interval between these two spectrums was 90 minutes, fill 1).

38
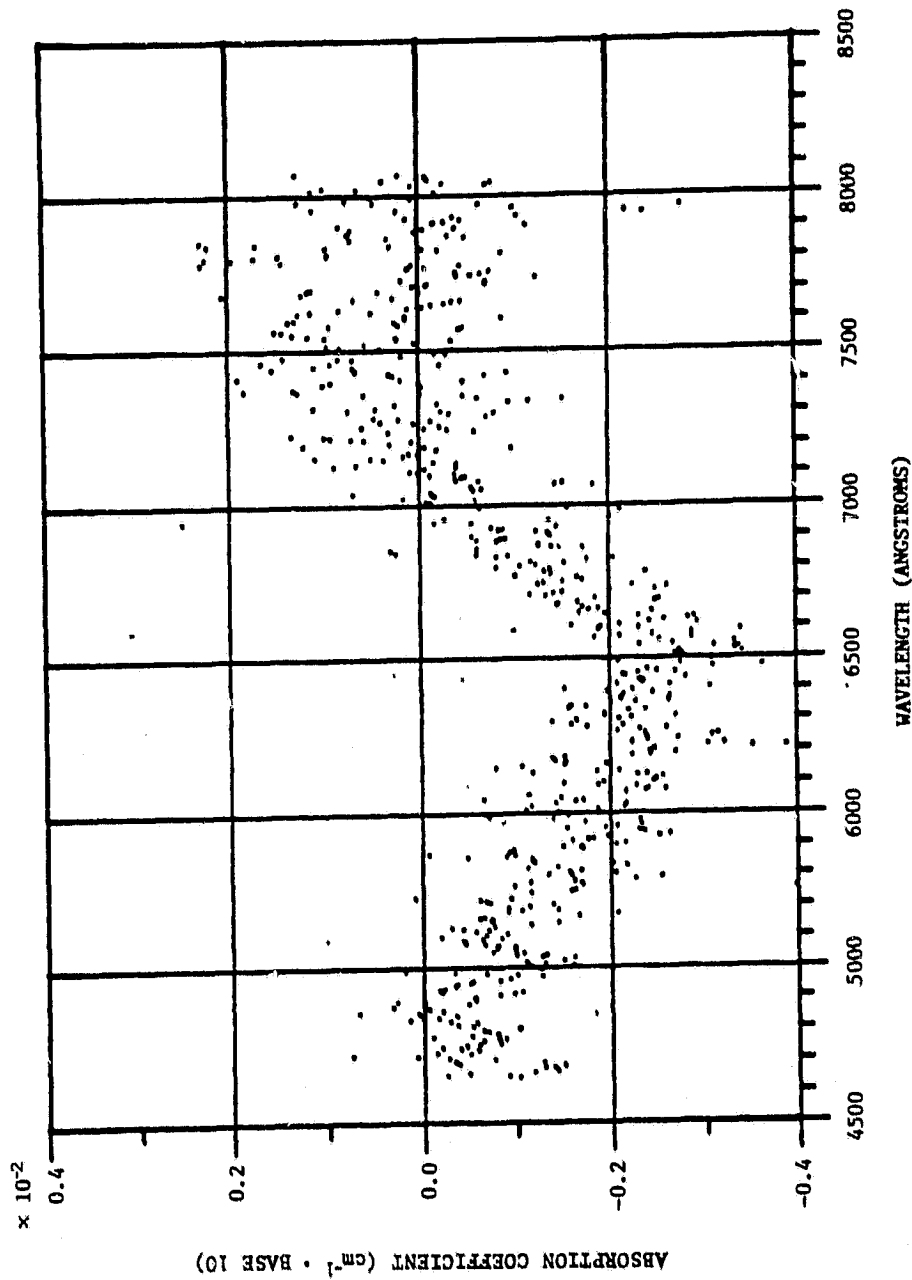
Figure 14. Difference of absorption spectrum when temperature was decreased from 303 K to 165 K (fill 1).
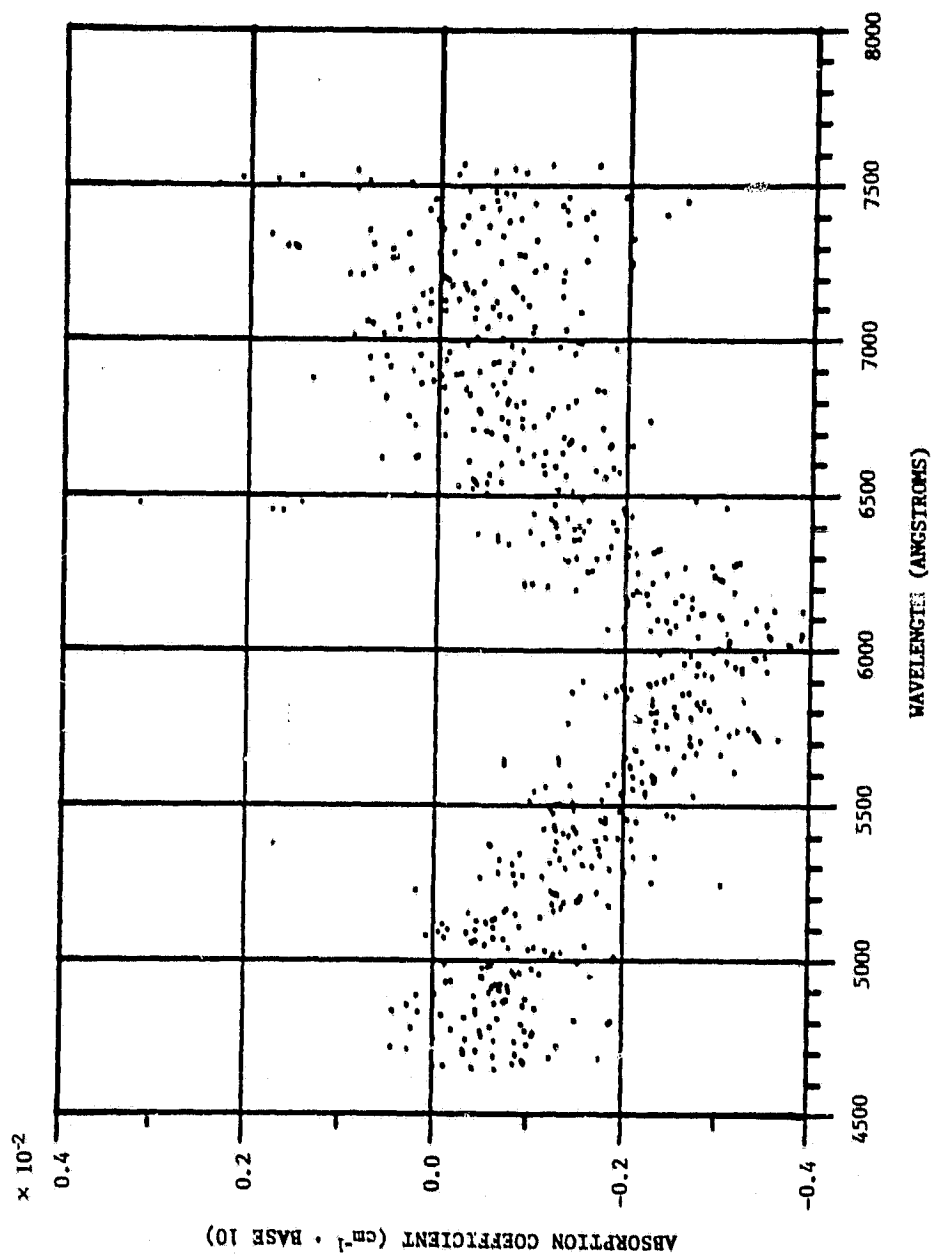
Figure 15. Difference of absorption spectrum when temperature was
increased from 165 K to 303 K (fill 1).
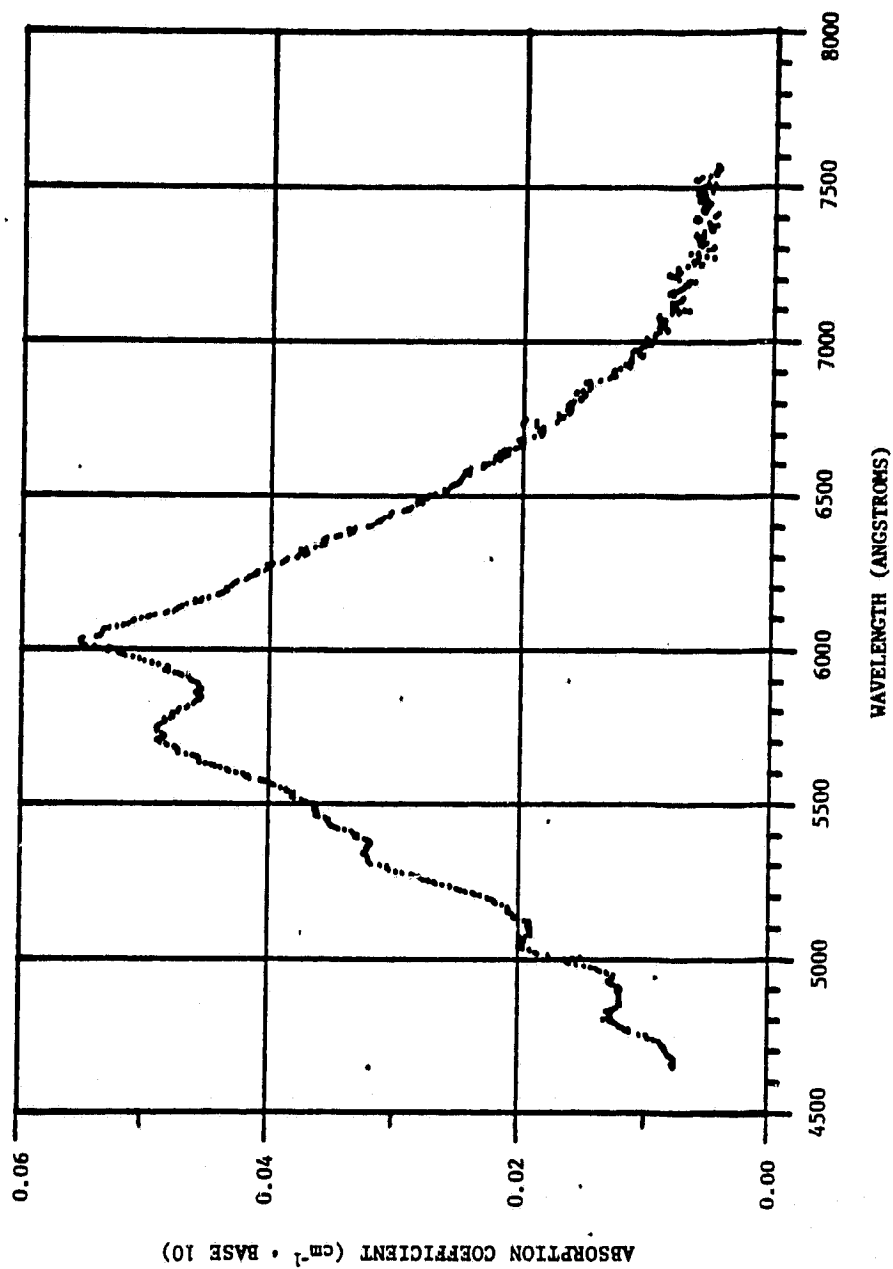
Figure 16. Calculated absorption spectrum of ozone at STP using a gas sample which was at T = 303 K and P = 37 cm Hg (fill 2).
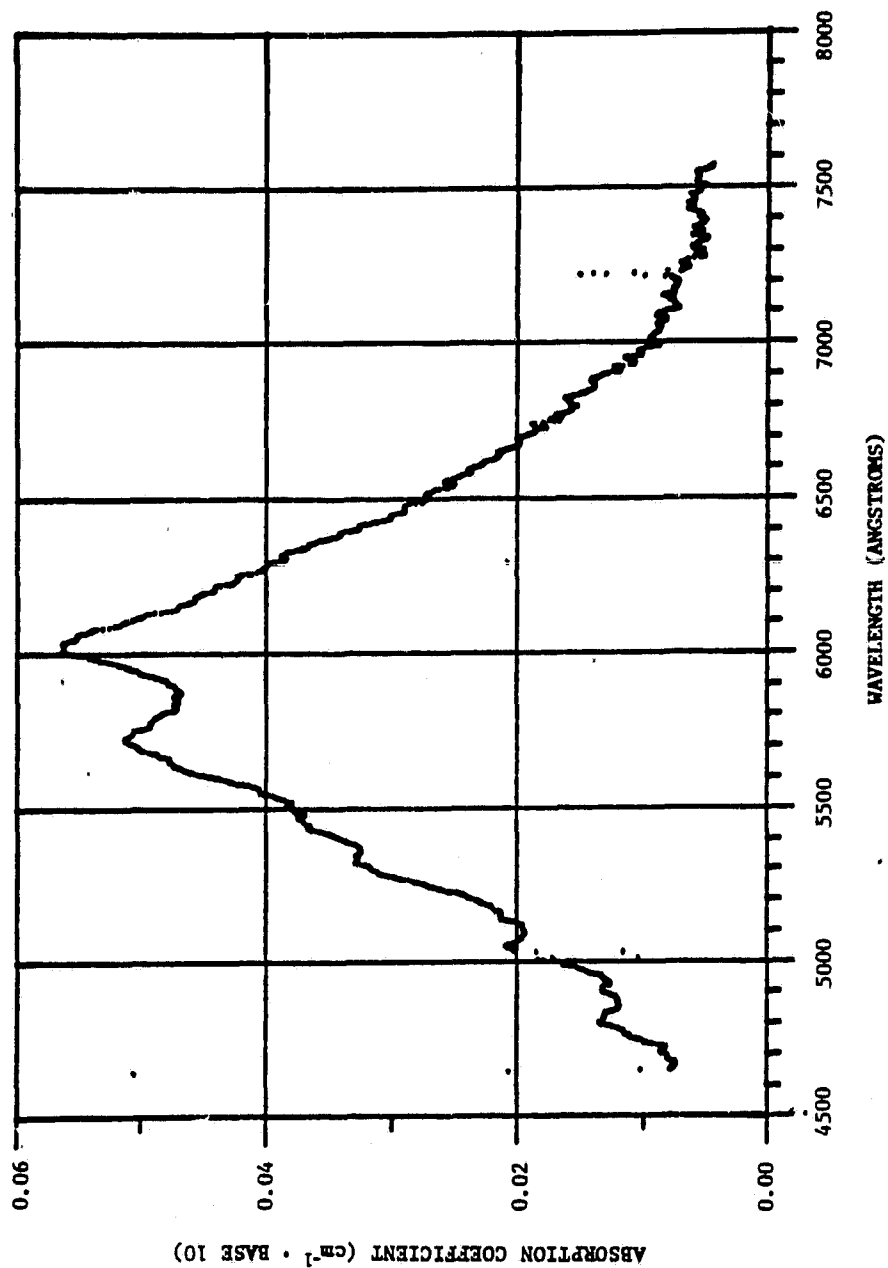
Figure 17. Calculated absorption spectrum at STP (40 minutes after filling) at T = 198 K (fill 2).

42
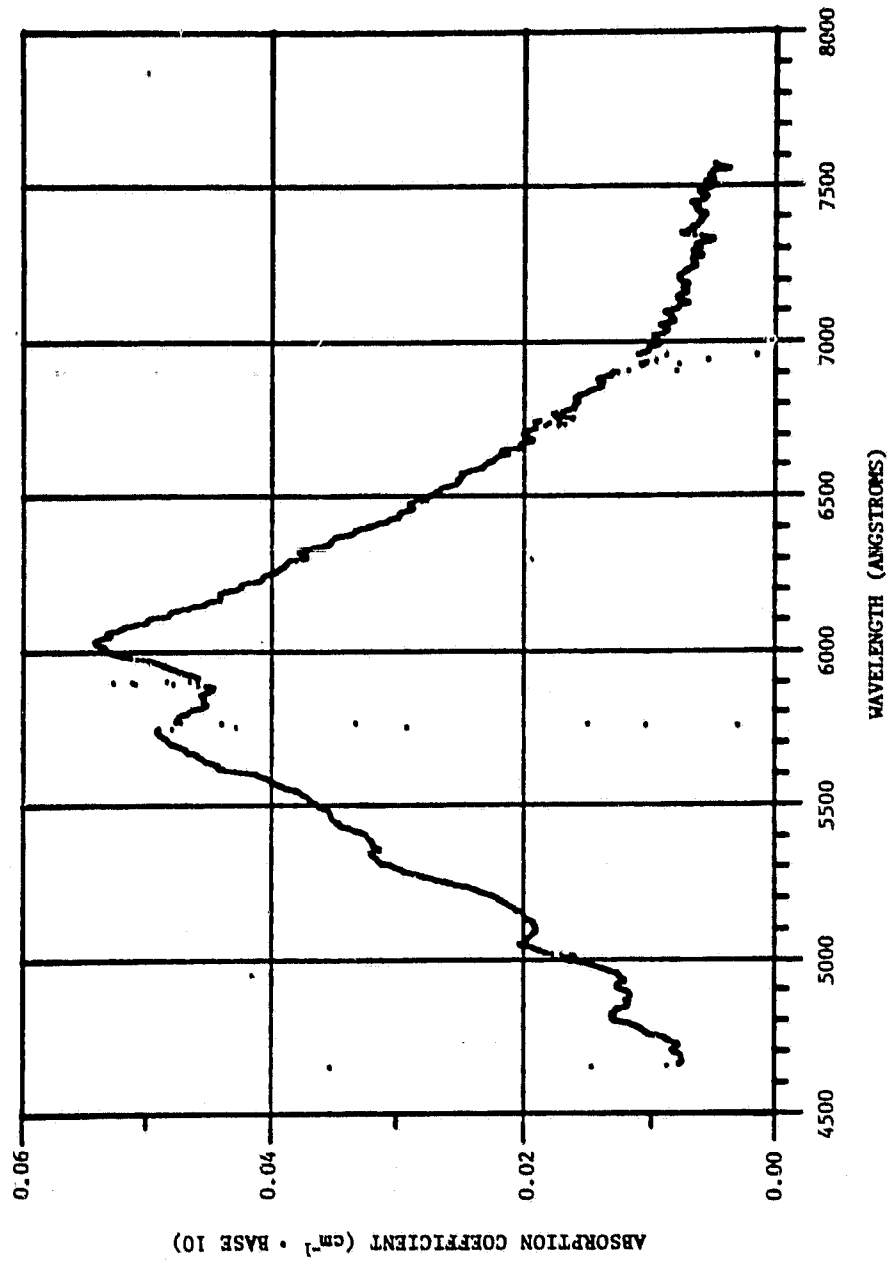
Figure 18. Calculated absorption spectrum at STP (60 minutes after filling) at T = 303 K (fill 2).

43
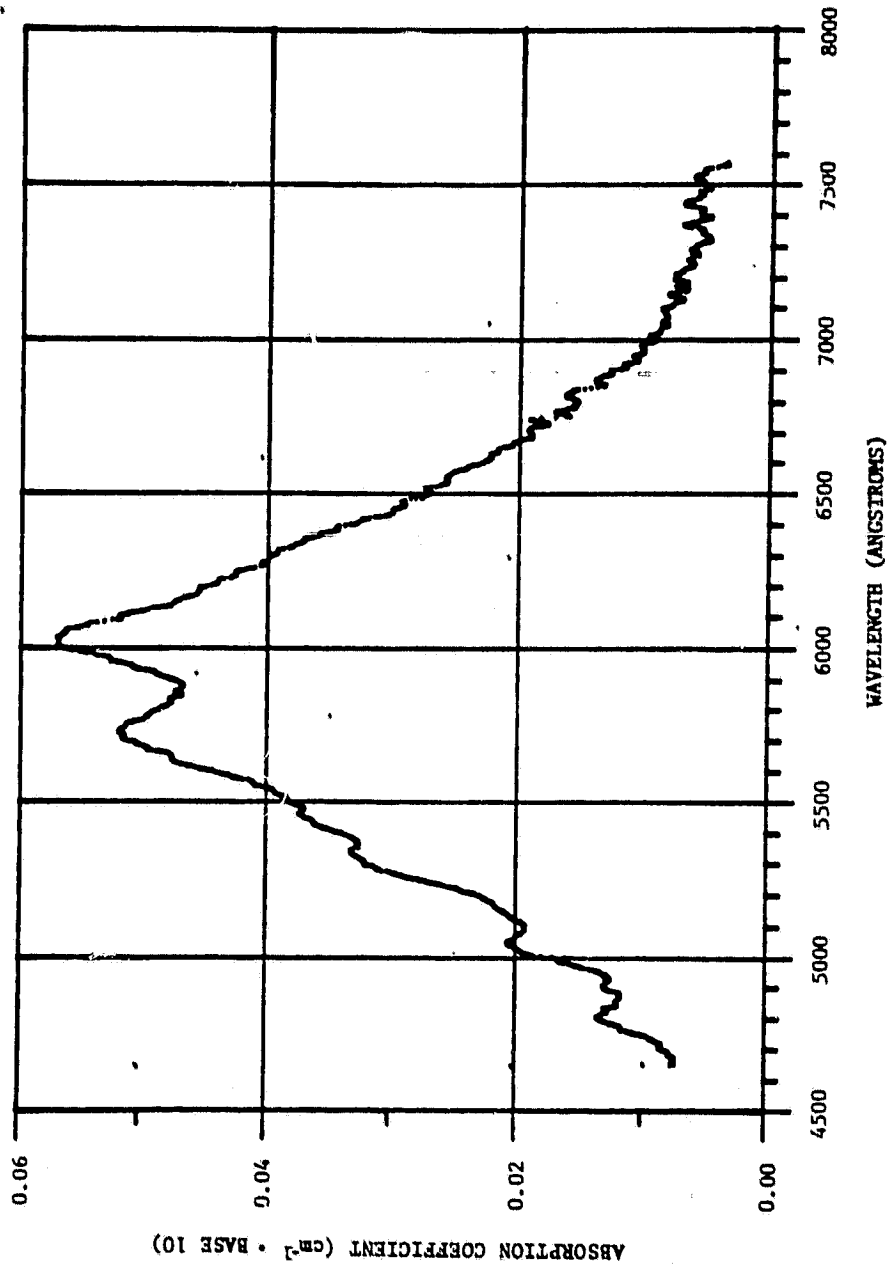
Figure 19. Calculated absorption spectrum at STP (2 hours after filling) at T = 165 K (fill 2).

44
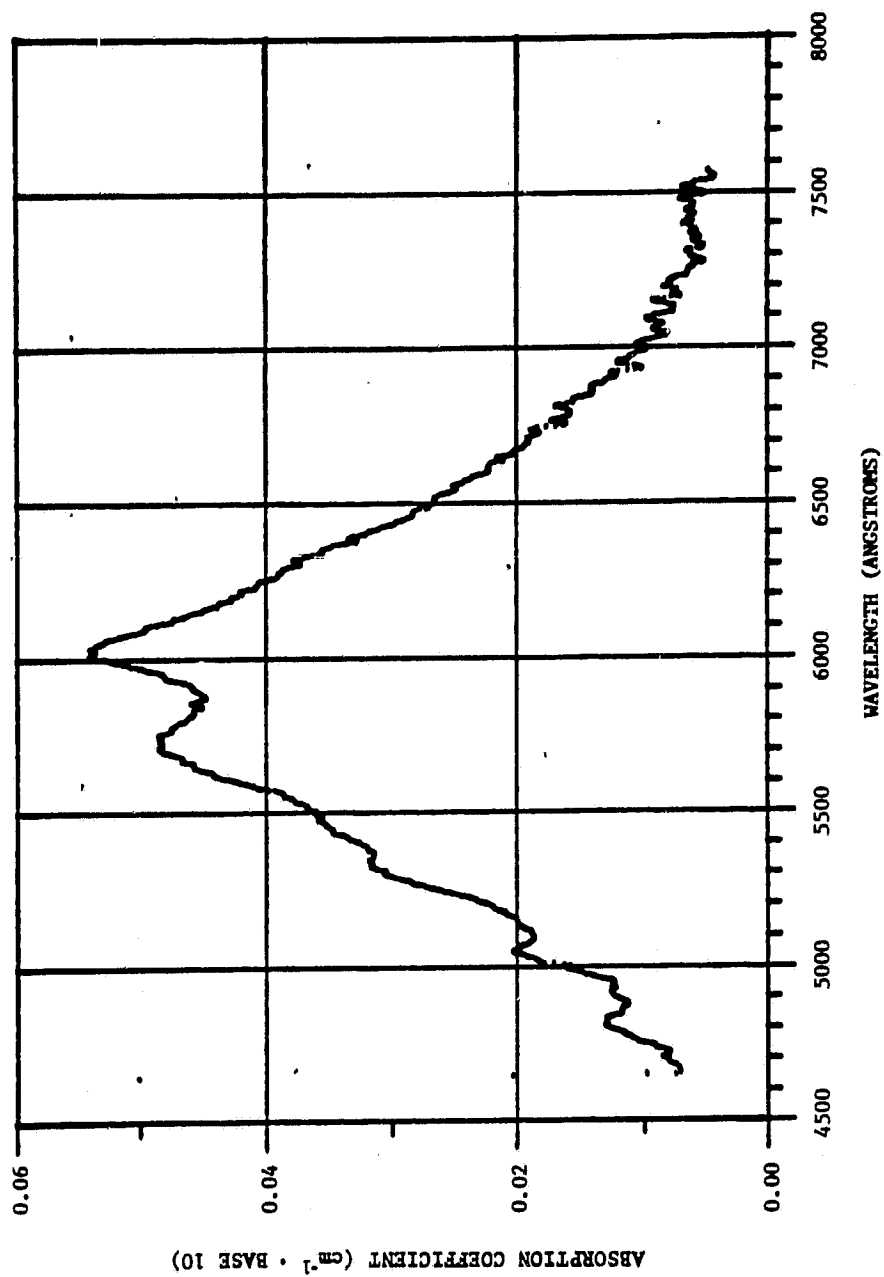
Figure 20. Calculated absorption spectrum at STP (about 3 hours after filling) at 303 K (fill 2).

45
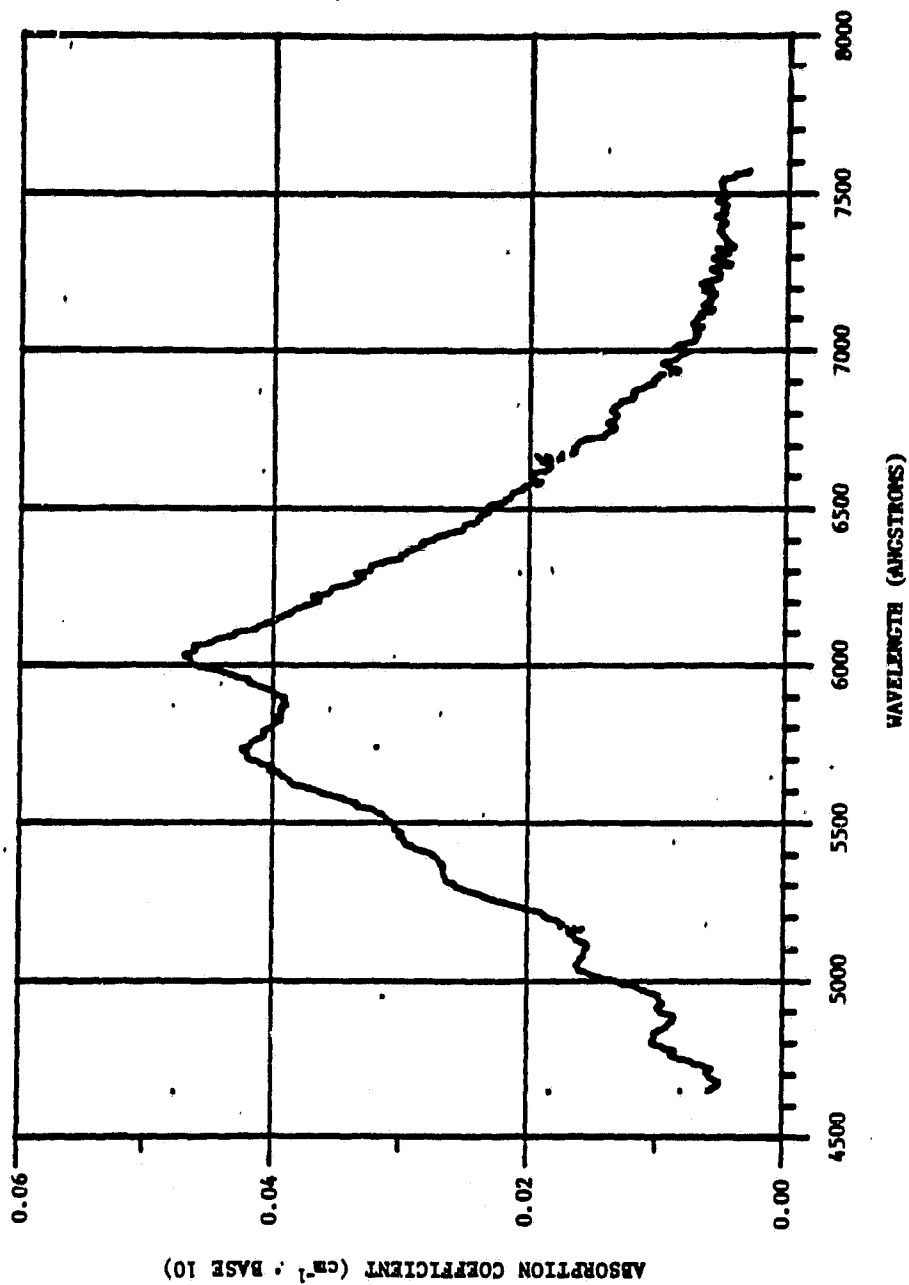
Figure 21. Calculated absorption spectrum at STP (about 43 hours after filling) at T = 303 K (fill 2).
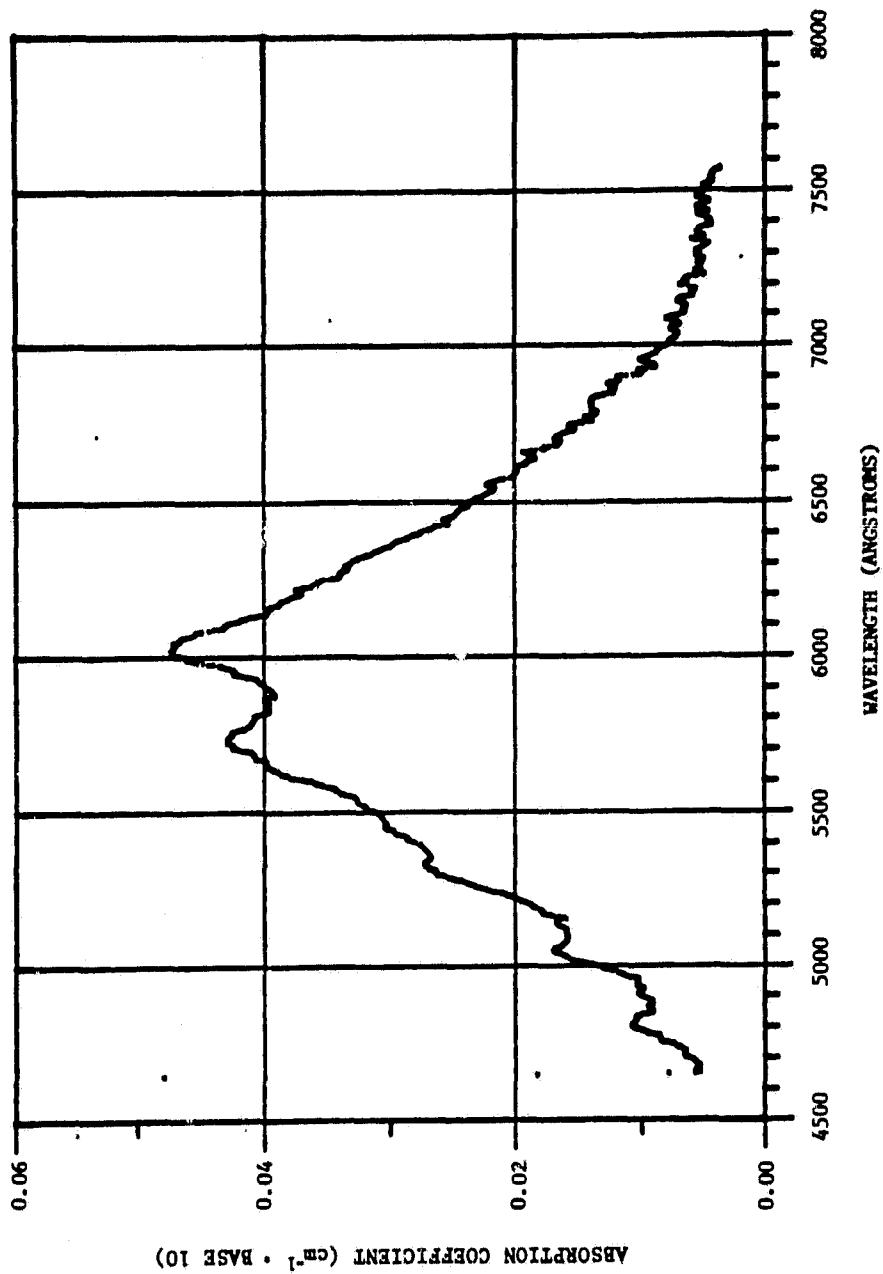
Figure 22. Calculated absorption spectrum at STP (44 hours after filling) at T = 303 K (fill 2).
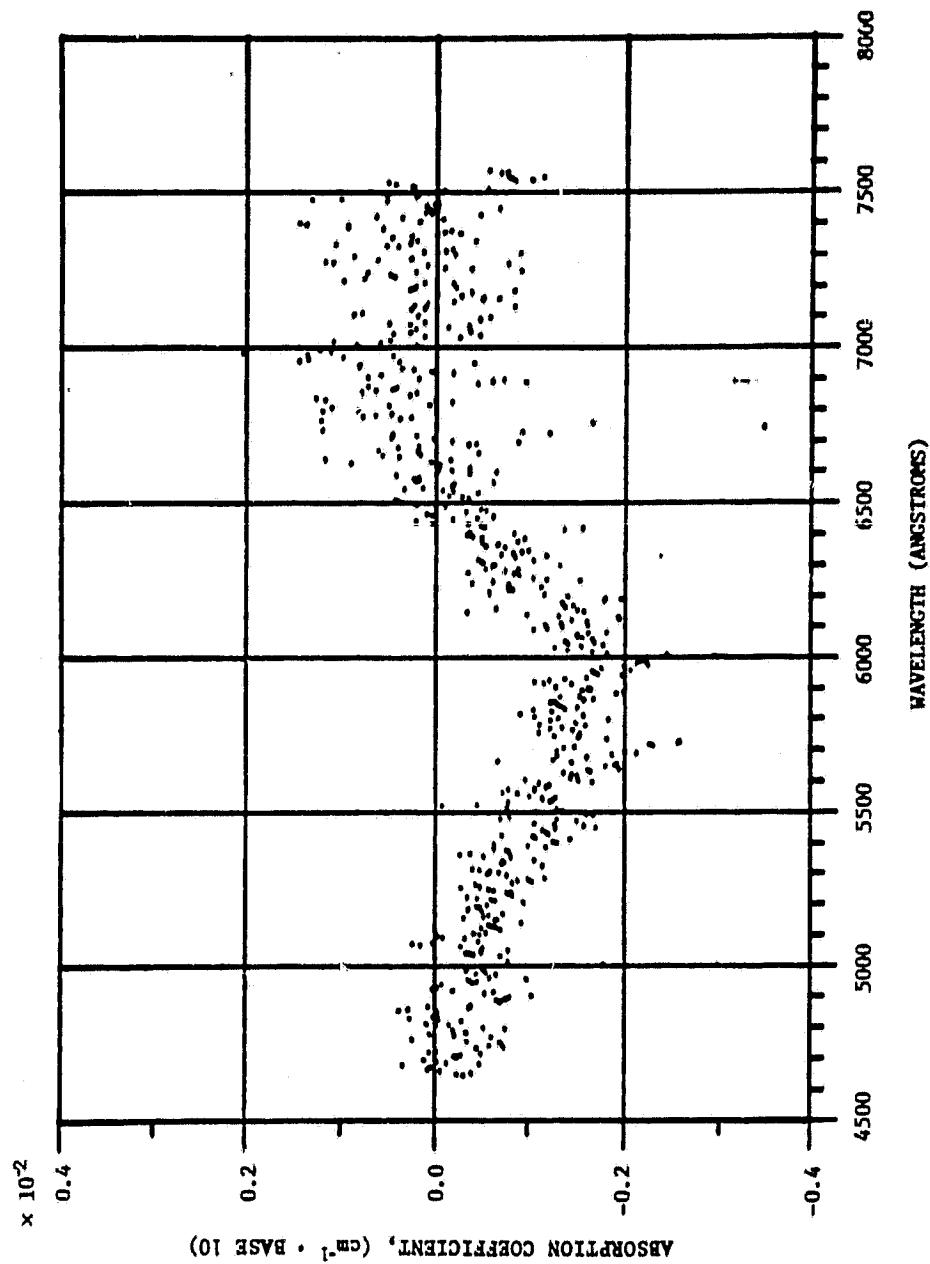
Figure 23. Difference of absorption coefficients when temperature was reduced from 303 K to 298 K (time interval between these two spectrums was about 35 minutes, fill 2).
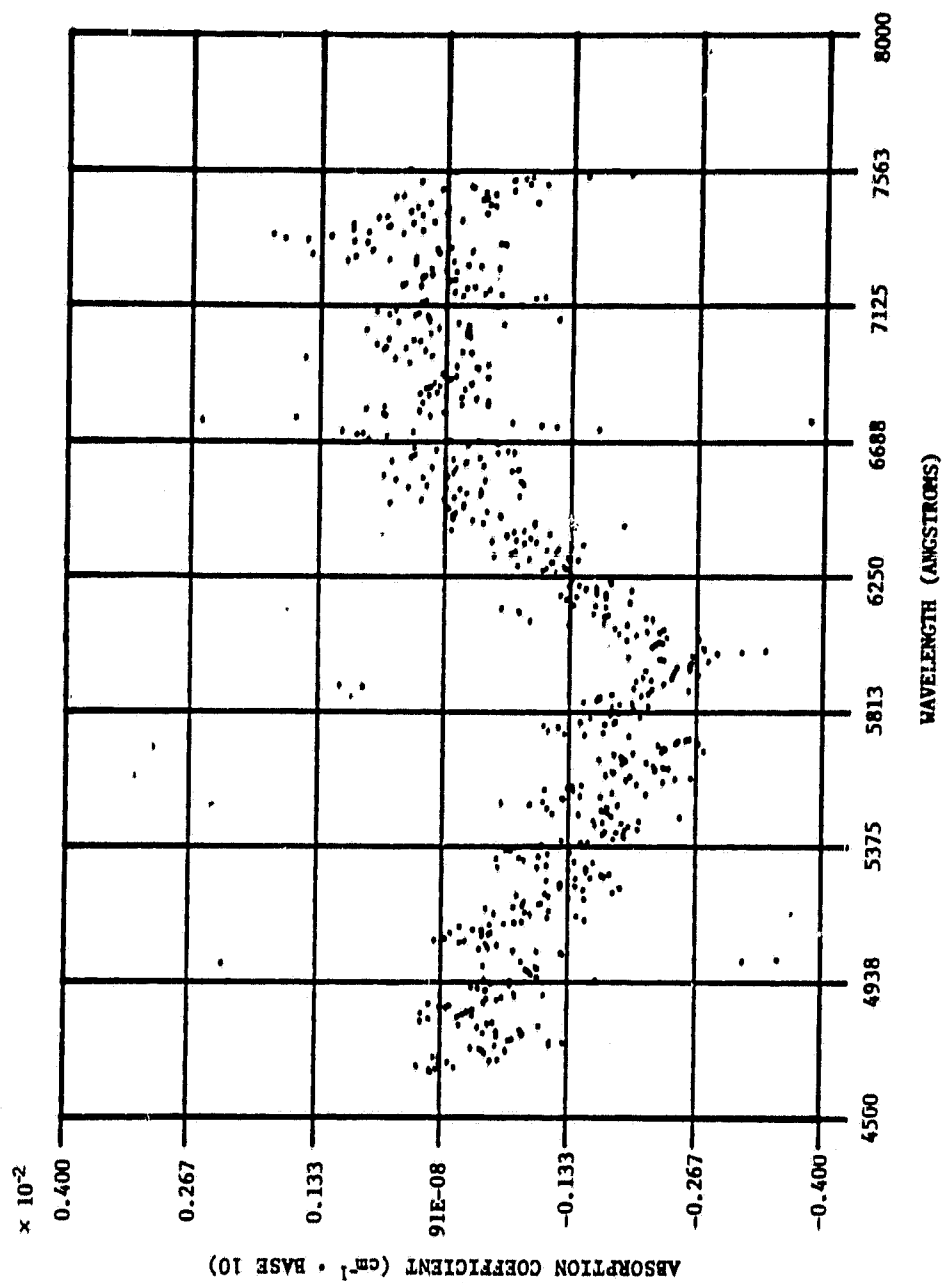
Figure 24. Difference of absorption spectrum when temperature was increased from 198 K to 303 K (time interval between these two spectrums was about 20 minutes, fill 2).
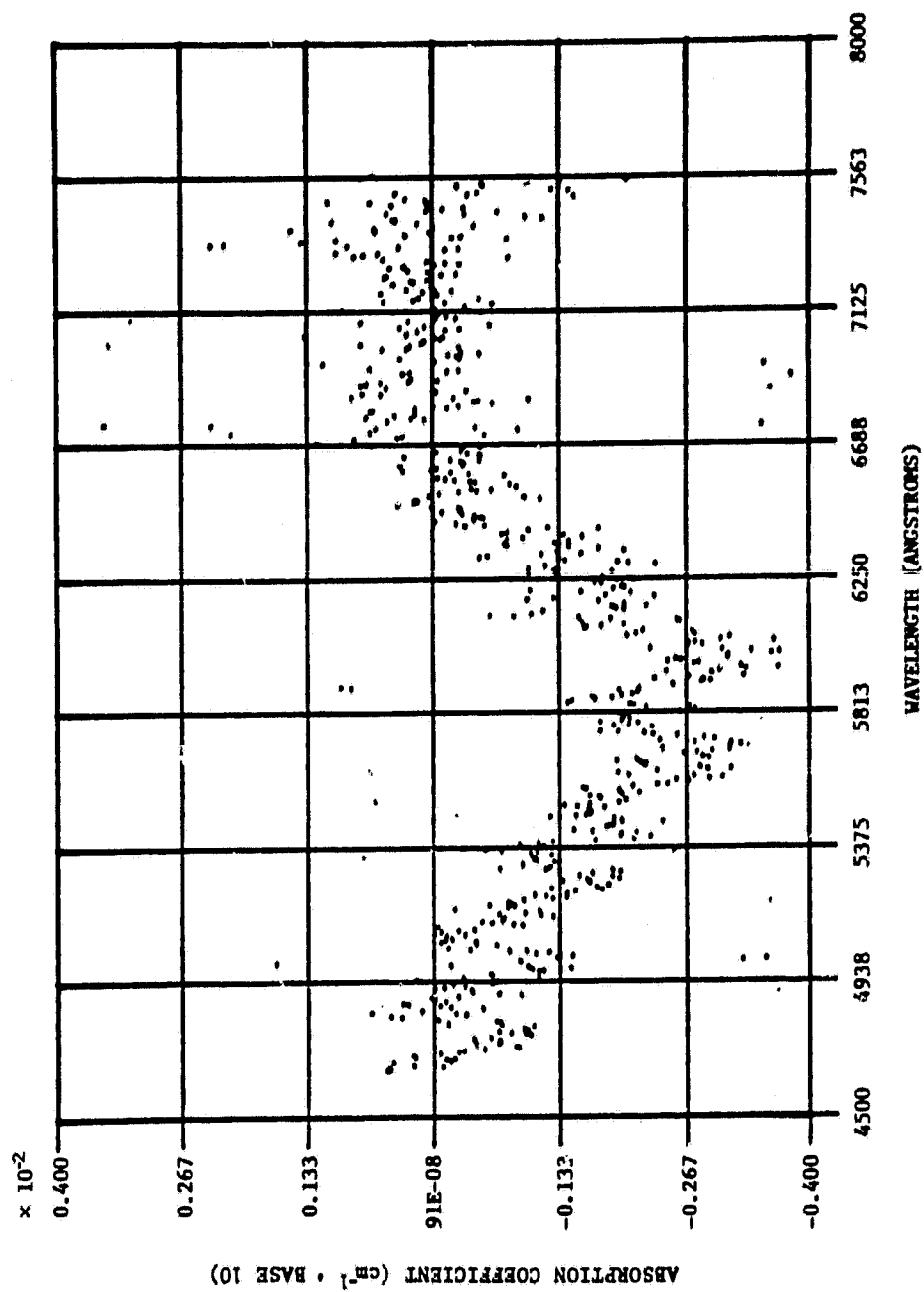
Figure 25. Difference of absorption spectrum when temperature was decreased from 303 K to 165 K (time interval between these two spectrums was about 60 minutes, fill 2).
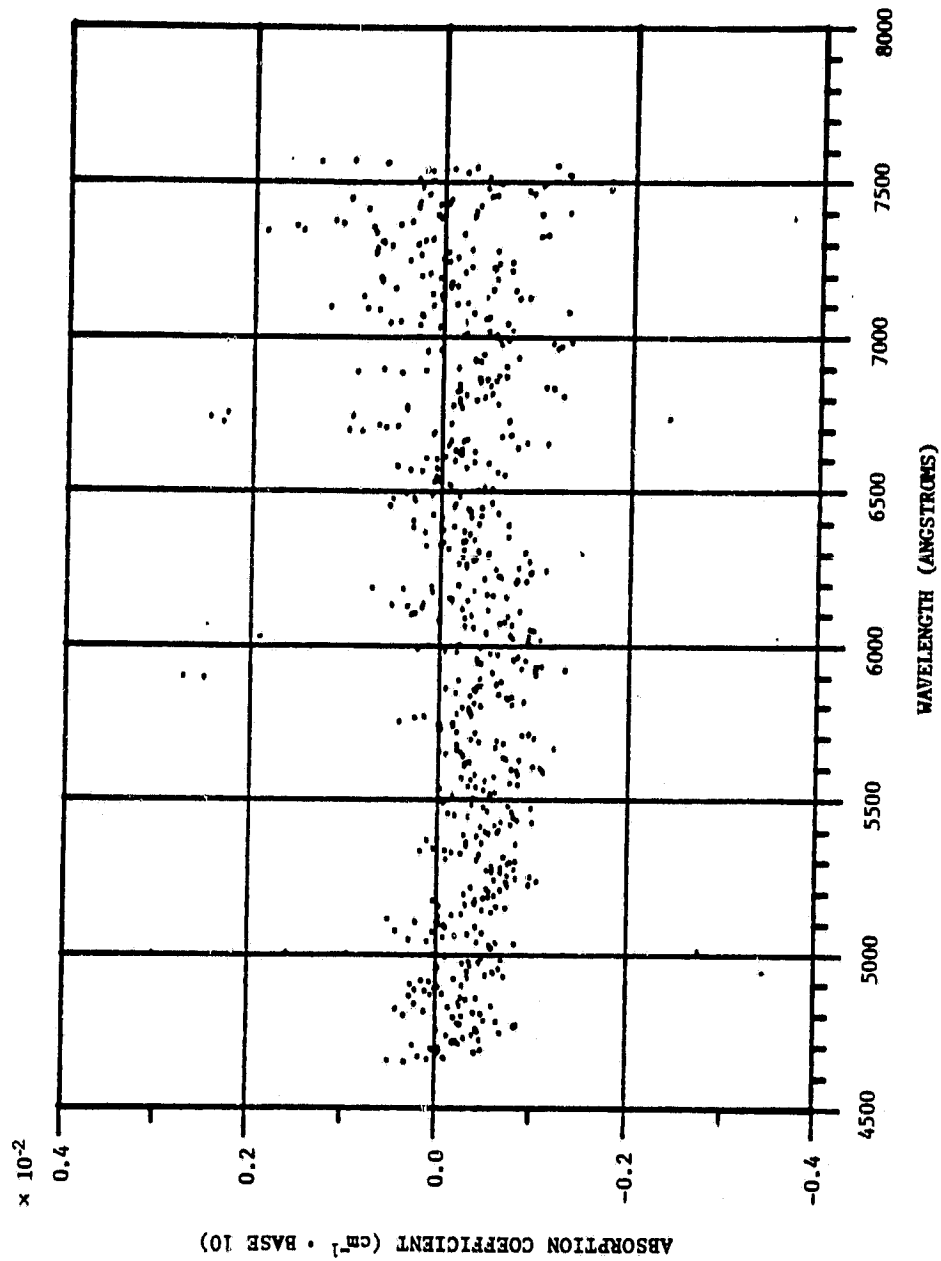
Figure 26. Difference in absorption coefficients after one temperature cycle at 303 K (time interval between these two spectrums was 60 minutes, fill 2).
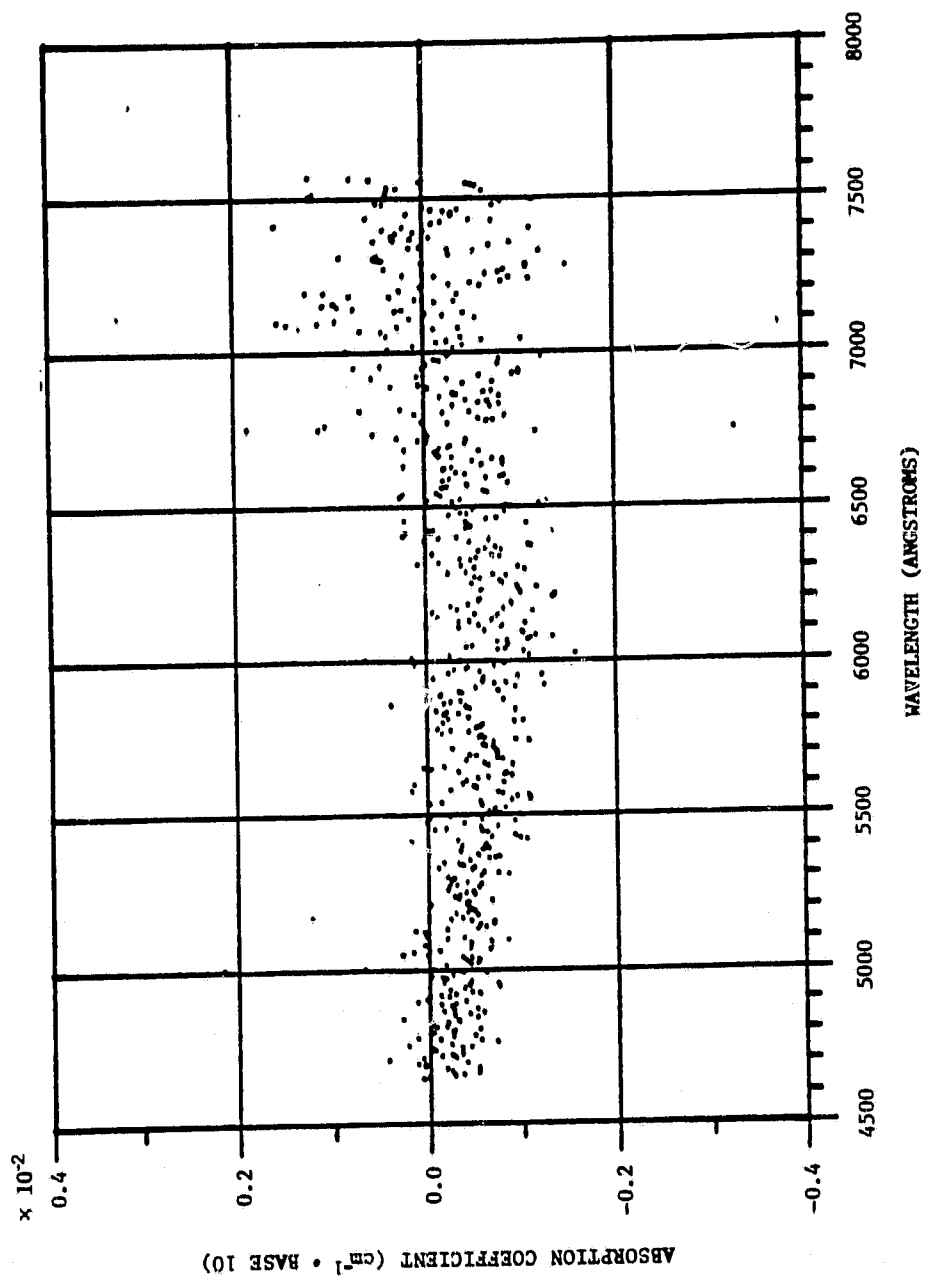
Figure 27. Difference in absorption coefficients after two temperature cycles at T = 303 K (time interval between these two spectrums was about 3 hours, fill 2).

52
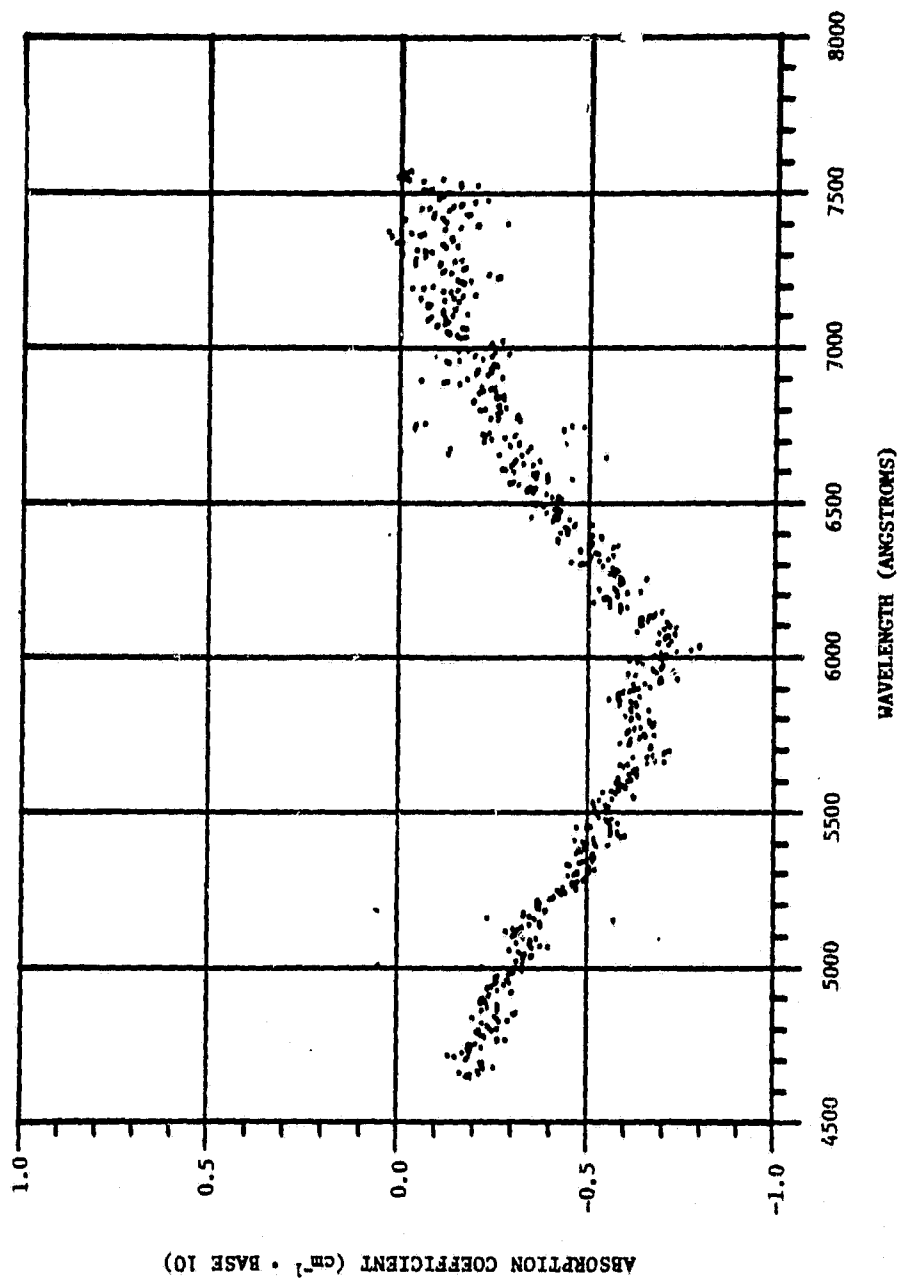
Figure 28. Difference in absorption coefficients after two temperature cycles at T = 303 K (time interval between these two spectrums was 44 hours, fill 2).

53
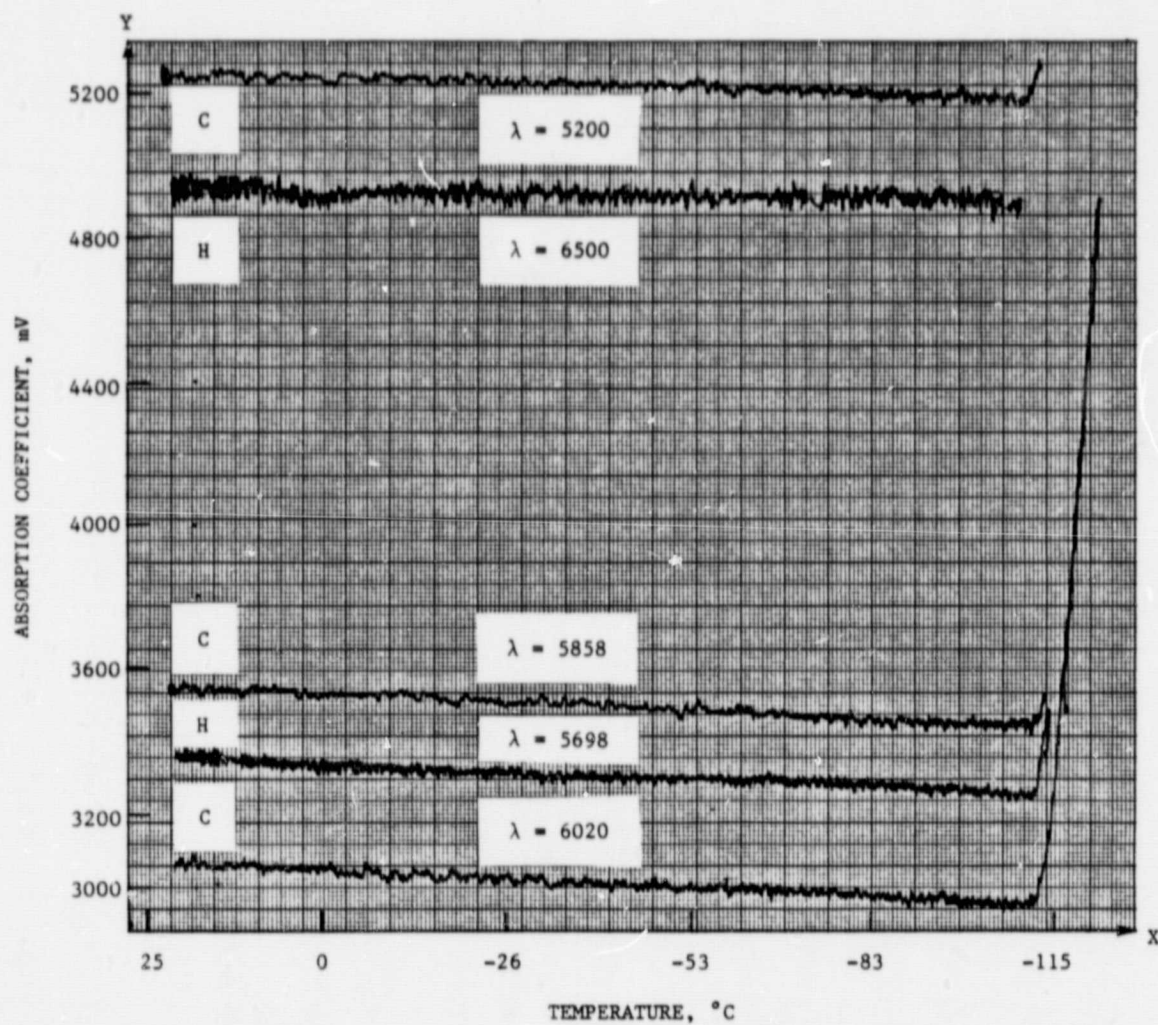
Figure 29. Variation of absorption coefficients for fixed
wavelengths as a function of temperature. C
and H designate cooling and heating of the gas
sample during the experiment.

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APPENDIX A

APPENDIX A

PROGRAM ADC

This program accepts anolog input originating from Perkin-Elmer Model 200 and creates a disk file on drive B:. The data containes 6000 blocks with one sample per block. These files were transfered to Dec-10 time shared computer, where the data was converted into decimal numbers.

```
;
;
;
BEGIN:  MVI     A,2H
        STA     FCB             ; DISK B AS DATA DISK
        CALL    INIT            ; INIT MEMORY LOCN'S
        CALL    PROMT
        CALL    CHECK           ; SEE IF FILE IS THERE
MAIN:   CALL    INLINE          ; TEXT LINE AT START
        CALL    CALIB
        CALL    DATIME          ; GET THE TIME
        CALL    INPT
        CALL    SETSZ           ; COMPUTE FILE SIZES
        CALL    FILE
        CALL    MORE
        JRZ     MAIN
        JMP     NUL             ; RETURN TO CPM
;
;       *** PROMPT THE USERS ***
;
PROMT:  LXI     D,MSG           ; "# OF CHANNELS"
        CALL    OUTSTR
        CALL    ECHO
        SBI     30H
        CPI     1H
        JM      PROMT
        CPI     3H
        JP      PROMT
        STA     CNT
        STA     NUM
        CALL    ECHO
        CPI     CR
        JRNZ    PROMT
        XRA     A
        STA     SEE
PRMA:   LXI     D,MSG0          ; SAMPLES / BLOCK(CH 0)
        CALL    OUTSTR
        CALL    INUM
        JM      PRMA
        LXI     D,SIZE
        XCHG
```

```
            CALL    SAVEN2
PRMB:       LXI     D,MSG1              ; # OF BLOCKS
            CALL    OUTSTR
            CALL    INUM
            JM      PRMB
            LXI     D,NUMBLK
            XCHG
            CALL    SAVEN2
PRMC:       LXI     D,MSG3              ; # STEPS PER BLOCKS ??
            CALL    OUTSTR
            CALL    INUM
            JM      PRMC
            CALL    SETSTP             ; CALCULATE PULSES/STEP
            LXI     H,STEPS
            CALL    SAVEN2
PRM1:       LXI     D,MSG2              ; SAMPLES PER CHAN(1)
            CALL    OUTSTR
            CALL    INUM
            JM      PRM1
            CALL    SETIM
            LXI     H,CST0
            CALL    SAVEN2
            LDA     CNT
            CPI     1                   ; ONLY ONE ?
            JRZ     PRM3
PRM2:       LXI     D,MSGE              ; SAMP..SEC..(25 MAX).
            CALL    OUTSTR
            CALL    INUM
            JM      PRM2
            CALL    SETIM               ; COMPUTE
            LXI     H,CST1
            CALL    SAVEN2
PRM3:       XRA     A
            STA     SLOW
            STA     SEE
            LXI     D,MSGS              ; FAST/SLOW MONITOR ??
            CALL    OUTSTR
            CALL    ECHO
            CPI     'S'
            CZ      SETSLO              ; MUST BE SLOW MON
            CALL    ECHO
            CPI     CR
            JRNZ    PRM3
PRM4:       LXI     D,MSGT
            CALL    OUTSTR              ; WANT TO WATCH ?
            CALL    ECHO
            CPI     'Y'
            CZ      SETSEE
            CALL    ECHO
            CPI     CR
            JRNZ    PRM4
PRM5:       LXI     D,MSGA              ;TYPE 'B' TO BACKUP
                                        ;..OR 'F' FORWARD...
                                        ; .. <RETURN> TO EXIT
            CALL    OUTSTR
            CALL    ZERO
            RET
SETSLO:     STA     SLOW
            RET
SETSEE:     STA     SEE
```

```
          RET
;
;
;         **** SAVE THE RESULT IN MEM ****
;
SAVEN2:   CALL    SAVEN
SAVEN:    MOV     M,E                 ; LOW ORDER BYTE FIRST
          INX     H
          MOV     M,D
          INX     H
          RET
;
;
;         **** CHECK FOR MORE FILES ****
;
MORE:     LXI     D,MSGR              ; "MORE ? "
          CALL    OUTSTR
          CALL    ECHO
          CPI     'N'                 ; NOPE ??
          JRZ     MCHEC
          CPI     'Y'
          JRNZ    MORE
          CALL    ECHO
          CPI     CR
          JRNZ    MORE
          LDA     NUM
          STA     CNT
          LXI     D,MSGB              ; RETURN LOCN OR NEW ?
          CALL    OUTSTR
          CALL    ECHO
          CPI     CR
          CNZ     ZERO                ; ??
          CZ      RTURN
          LHLD    NUMBLK+2
          SHLD    NUMBLK              ; RESTORE FILESIZE
          CALL    INIT
          CALL    INFLO               ; GET NEW FILENAME
          XRA     A
          RET
MCHEC:    CALL    ECHO
          CPI     CR
          JRNZ    MORE
          DCR     A
          RET                         ; NON ZERO
;
;
;         **** CALIBRATE THE A TO D CONVERTER ****
;
CALIB:    MVI     A,NUL
          STA     UNI
          LXI     D,MSG4              ; "UNIPOLAR OR BIPOLAR"
          CALL    OUTSTR
          CALL    ECHO
          CPI     'B'
          CZ      SETUNI              ; -1 = BIPOLAR
          CPI     'U'
          JRNZ    CALIB
          CALL    INCH
          CPI     CR
          JRNZ    CALIB
```

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```
            LDA     UNI
            ORA     A
            JM      ETC             ; BIPOLAR
            LXI     D,MSG5          ; SWITCH TO THE LEFT
            MVI     B,7H
            CALL    CALP
            LXI     D,MSG7          ; LEFT POT TO '01FF'
            MVI     B,6H
            JMPR    CALP
ETC:        LXI     D,MSG8          ;   SWITCH TO THE RIGHT
            MVI     B,7H
            CALL    CALP
            LXI     D,MSG10         ; LEFT POT TO '03FF'
            MVI     B,6H
            JMPR    CALP
;
;
SETUNI:     CMA                     ; SET TO -1
            STA     UNI
            MVI     A,'U'           ; FAKE OUT REST
            RET
;
;
CALP:       CALL    OUST
            CALL    LOOP
            IN      DAT
            RET
;
;
LPT1:       IN      STAT
            ANI     2H
            RNZ
LOOP:       MVI     A,CR            ; CALL W/ CHAN # IN 'B'
            CALL    OUCH
            MOV     A,B
            OUT     DSTAT
            NOP
LP1:        IN      DSTAT
            RRC
            JRC     LP1
            NOP
            IN      DDAT
            MOV     C,A
            NOP
            IN      DDAT
            ANI     03H
            CALL    CNVERT
            MOV     A,C
            CALL    CNVERT
            LDA     SLOW
            ORA     A
            JRZ     LPT1
            MVI     A,LF
            CALL    OUCH
            CALL    INCH
            CPI     CR
            RZ
            JMPR    LOOP
;
;
```

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```
CNVERT: PUSH      PSW
        RRC
        RRC
        RRC
        RRC
        CALL      VERT
        POP       PSW
VERT:   ANI       0FH
        ADI       30H
        CPI       3AH
        CP        ABIAS
        CALL      OUCH
        RET
ABIAS:  ADI       7H
        RET
;
;
;       **** INSERTING TEXT AT THE BEGINNING ****
;
INLINE: LXI       H,TXTBUF
        LXI       D,MSGL
        CALL      OUST
        MVI       C,0         ; POSITION COUNTER
TXTLP:  CALL      ECHO
        CPI       7FH         ; <RUBOUT>
        JRZ       BACUP
        CPI       08H         ; <©H>
        JRZ       BACON
        CPI       18H         ; <ESC>
        JRZ       INLINE
        MOV       M,A
        INX       H
        INR       C
        CPI       CR
        JRNZ      TXTLP
        MVI       A,LF
        CALL      OUCH
        MOV       M,A
        INX       H
        MVI       M,26        ; <©Z>
        INR       C
        INR       C
        MVI       H,0
        MOV       L,C
        SHLD      TXTSZ
        SHLD      TXTSZ2
        RET
;
;
BACON:  DCR       C
        JM        INLINE
        DCX       H
        JMPR      TXTLP
BACUP:  DCR       C
        JM        INLINE
        DCX       H
        MOV       A,M
        CALL      OUCH
        JMPR      TXTLP
;
```

```
;
;
;       **** CREATING THE DISK FILE ****
;
FILE:   CALL    SETUP
        LXI     D,START0
        LHLD    SHL0
        CALL    RITE
        RZ
        CALL    SETUP
        LXI     D,START1        ; START OF FILE BLOCK 1
        LHLD    SHL1            ; FILE 1 SIZE
        JMP     RITE            '
;
;
;       **** CHECKING FOR A FILE ALREADY THERE ****
;
CHECK:  LDA     FCBFN           ; LOOK AT FILENAME
        CPI     ' '
        JRZ     INFL0           ; GET ONE
        CALL    DFIND
        CALL    CLRFN
        INR     A
        RZ
        CALL    CRLF
        LXI     D,MSGF          ; RENAME NEW FILE ??
        CALL    OUTSTR
        CALL    ECHO
        CPI     59H             ; 'Y'
        JRZ     INFILE
        CALL    CRLF
        LXI     D,MSGW          ; WARN THE SUCKER
        CALL    OUTSTR
        CALL    ECHO
        CPI     59H             ; HES SURE ??
        JRNZ    INFILE          ; NOPE
        CALL    INCH            ; GET <CR>
        CPI     CR
        JRNZ    INFILE          ; MUST NOT BE SURE
        CALL    DERASE          ; ELSE ERASE IT
        CALL    CLRFN
        RET
;
;
INFILE: CALL    INCH
        CPI     CR
        JRNZ    CHECK
INFL0:  LXI     H,FCB+1
        MVI     B,12
        CALL    SETBLK
        CALL    CLRFN
        CALL    CRLF
        LXI     H,FCB+1
        LXI     D,MSGQ          ; NEW FILENAME :
        CALL    OUTSTR
INFL1:  CALL    ECHO
        CPI     7FH             ; RUBOUT ??
        JRZ     INFL0
        CPI     2EH             ; '.'
        JRZ     INFL2
```

```
            CPI       CR
            JRZ       CHECK
            MOV       M,A
            INX       H
            JMPR      INFL1
INFL2:      LXI       H,FCB+9
            MVI       B,3
INFL3:      CALL      ECHO
            CPI       7FH
            JRZ       INFLC
            CPI       CR
            JRZ       CHECK
            MOV       M,A
            INX       H
            DCR       B
            JRNZ      INFL3
            CALL      INCH
            CPI       CR
            JRNZ      INFLO
            JMP       CHECK
;
;
;           **** CLEAR THE GARBAGE AT END OF FCB ****
;
CLRFN:      PUSH      PSW
            MVI       B,21
            LXI       H,FCB+12
            CALL      CLRBLK
            POP       PSW
            RET
;
;
;           **** SETTING FILE SIZES ****
;
SETSZ:      LXI       D,MSGP
            CALL      OUST
            LXI       D,SIZO+1
            LXI       H,SHLO+1
            MOV       A,M
            SBI       OFFO
            CALL      CALCSZ
            SBI       OFF1
CALCSZ:     MOV       M,A
            MOV       B,A
            XRA       A
            MOV       A,B
            RAR                 ; DIV BY 2 HI BYTE
            STAX      D
            DCX H
            DCX D
            MOV       A,M
            RAR                 ; LO BYTE
            STAX      D
            INX H
            INX H
            INX H
            INX D
            INX D
            INX D
            MOV       A,M
```

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```
          RET
;
;
;         **** SET UP FOR DISK WRITES ****
;
SETUP:    CALL    DMAKE                 ; CREATE THE FILE
          INR     A
          JZ      CRERR
          CALL    DOPEN                 ; OPEN IT
          INR     A
          JZ      FLERR
          RET
;
;
;         **** WRITING TO THE DISK ****
;
RITE:     CALL    HEADER
          JMPR    RITE2
RITE1:    LXI     H,BUFF
          MOV     A,L
          STA     BLKSZ                 ; SIZE OF BLOCK
RITE2:    CALL    BLK                   ; TRANSFER THE BLOCK
          JRC     DONE
          PUSH    B
          PUSH    D
          CALL    DWRIT
          ORA     A
          JNZ     WRER
          POP     D
          POP     B
          JMPR    RITE1
DONE:     XRA     A
          SUB     L
          MOV     B,A
          CALL    CLRBLK
          CALL    DWRIT
          CALL    DCLOS
          CALL    UPFILE                ; UPDATE FILENAME
          CALL    CLRFN
          LDA     CNT
          DCR     A
          STA     CNT
          RET
;
;
;         *** UPDATING THE FILENAME ****
;
UPFILE:   LDA     FCB+6    ; *****?.***
          INR     A
          CPI     ':'      ; OVERFLOW ?
          CZ      UPFL1
          STA     FCB+6
          RET
UPFL1:    LDA     FCB+5    ; ****?*.***
          INR     A
          CPI     ':'      ;
          CZ      UPFL2
          STA     FCB+5
          MVI     A,'0'
          RET
```

```
UPFL2:  LDA     FCB+4     ; ***?**.***
        INR     A
        CPI     ';'
        JZ      CRERR     ; TOO MANY !!
        STA     FCB+4
        MVI     A,'0'
        RET
;
;
;
;       **** DISK FILE TRANSFER ****
; ... SOURCE <DE> ... DESTINATION <HL> ...
; .. LENGTH "BLKSZ" ... FILE SIZE <BC> ...
;
BLK:    LDA     BLKSZ
        DCR     A
        STA     BLKSZ
        JM      BLKQ
        LDAX    D
        MOV     M,A
        INX     H
        INX     D
        DCR     C
        JRZ     HIBLK
        MOV     A,C
        CPI     0FFH
        JRNZ    BLK
        DCR     B
        JMPR    BLK
HIBLK:  MOV     A,B
        ORA     A
        JRNZ    BLK
        STC
        RET
BLKQ:   XRA     A
        RET
;
;
;
;       **** INSERT HEADER INFO ****
;
HEADER: PUSH    H
        PUSH    D                 ; SAVE THE SOURCES
        LXI     H,BUFF            ; SET UP DEST ADDRS
        LXI     D,FCBFN           ; NAME + EXT
        MVI     B,11
        CALL    BLT
        MVI     B,3
        CALL    SETBLK
        CALL    TIMEX             ; DATE & TIME
        CALL    OFFSET
        RAL                       ; X 2
        LXI     D,SIZO
        CALL    FILNUM            ; # OF SAMPLES
        MVI     B,27
        LXI     D,SMPSC           ; SAMPLES.  SAMPLE PER.
        CALL    BLT
        LDA     OFST              ; OFFSET
        RAL
        RAL               ; X 4
        LXI     D,CSTO  ; CSTO+OFFSET = # CLOCKS/SAMPLE
```

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```
                    CALL      FILNUM
                    LXI       D,CLKDT          ; 3.3280 MS/CLOCK
                    MVI       B,20
                    CALL      BLT
                    XRA       A                ; NO OFFSET
                    LXI       D,SIZE           ; SAMPLES/BLOCK
                    CALL      FILNUM
                    LXI       D,DMSG
                    MVI       B,15
                    CALL      BLT
                    XRA       A
                    LXI       D,NUMBLK+2       ; BLOKS/RUN
                    CALL      FILNUM
                    MOV       A,L
                    CMA
                    INR       A
                    STA       BLKSZ
                    LXI       D,DM2
                    LXI       B,13
                    CALL      BLK
                    PUSH      H
                    LHLD      TXTSZ
                    MOV       B,H
                    MOV       C,L              ; BC - SIZE OF TEXTFILE
                    POP       D
                    LXI       H,TXTBUF
                    XCHG                       ; DE>DEST ... HL>SOURCE
                    CALL      BLK
                    CNC       TRITE
                    POP       D
                    POP       B
                    RET
OFFSET:  LDA        CNT
                    MOV       B,A
                    LDA       NUM
                    SUB       B
                    STA       OFST
                    RET
;
;
;         **** TEXT WRITING TO DISK ****
;
TRITE:   PUSH       B
                    PUSH      D
                    CALL      DWRIT
                    ORA       A
                    JNZ       WRER
                    POP       D
                    POP       B
                    LXI       H,BUFF
                    MOV       A,L
                    STA       BLKSZ
                    CALL      BLK
                    RC
                    JMPR      TRITE
;
;
;
;         **** TRANSFERRING A NUMBER TO FILE ****
;
```

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```
FILNUM: ADD     E
        MOV     E,A                 ; CORRECT OFFSET
        XCHG
        MOV     C,M                 ; DE-BUFF   HL-SRC OF #
        INX     H
        MOV     H,M
        MOV     L,C                 ; DE-BUFF   HL-#
        LXI     B,M10000
        CALL    FINUL
        LXI     B,10000
        DAD     B
        LXI     B,M1000
        CALL    FINUL
        LXI     B,1000
        DAD     B
        LXI     B,M100
        CALL    FINUL
        LXI     B,100
        DAD     B
        LXI     B,M10
        CALL    FINUL
        MOV     A,L
        ADI     3AH                 ; CORRECTION+ASCII '0'
        STAX    D
        INX     D
        XCHG
        RET
FINUL:  PUSH    D
        MVI     D,'0'
        DAD     B
        MOV     A,H
        ORA     A
        JM      FINUL2
        INR     D
        JMPR    FINUL+3
FINUL2: MOV     A,D
        POP     D
        STAX    D
        INX     D
        RET
;
;
;       **** INSERTING DATE & TIME IN FILE ****
;
DATIME: CALL    GET
        XRA     A
        STA     HH
        STA     MM
        STA     SS
        LXI     B,TT
        LXI     H,C8600
        CALL    SUBT
        LDA     H2
        ANI     80H
        JRNZ    NODAY
NEWDAY: LXI     H,DD
        INR     M
        CALL    SETHW
        JMPR    SUBHR
NODAY:  LXI     B,TT
```

```
            LXI     H,C8600
            CALL    ADDT
SUBHR:      LXI     B,TT
            LXI     H,C3600
            CALL    SUBT
            LDA     H2
            ANI     80H
            JRNZ    SUBPR
            LXI     H,HH
            INR     M
            JMPR    SUBHR
SUBPR:      LXI     B,TT
            LXI     H,C3600
            CALL    ADDT
SUBMI:      LXI     B,TT
            LXI     H,C60
            CALL    SUBT
            LDA     H2
            ANI     80H
            JRNZ    SUBSC
            LXI     H,MM
            INR     M
            JMPR    SUBMI
SUBSC:      LXI     B,TT
            LXI     H,C60
            CALL    ADDT
            LDA     TT
            STA     SS
            RET
;
;           ** MOVE TIME TO BUFFER **
;
TIMEX:      LXI     D,DD
            CALL    BINAS
            CALL    MONTH
            LXI     D,HH
            CALL    BINAS
            MVI     M,':'
            INX     H
            LXI     D,MM
            CALL    BINAS
            MVI     M,':'
            INX     H
            LXI     D,SS
            CALL    BINAS
            MVI     M,CR
            INX     H
            MVI     M,LF
            INX     H
            RET
;
;
ADDT:       MVI     E,3
            XRA     A           ; CLEAR CARRY
LOOPA:      LDAX    B
            ADC     M
            STAX    B
            DCR     E
            RZ
            INX     H
```

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```
            INX       B
            JMPR      LOOPA
;
;
SUBT:       MVI       E,3
            XRA       A
LOOPS:      LDAX      B
            SBB       M
            STAX      B
            DCR       E
            RZ
            INX       H
            INX       B
            JMPR      LOOPS
;
;
GET:        IN        T0
            STA       H0
            IN        T1
            STA       H1
            IN        T2
            STA       H2
            ANI       8H
            JRNZ      GET         ; NOT READY
            LDA       H2
            ANI       1H
            STA       H2
            RET
;
;
BINAS:      LDAX      D           ; GET TIME
            MVI       C,HUND
            MVI       D,0
            CALL      TCON
            INR       D
BA1:        MOV       A,E
            MVI       C,TEN
            CALL      TCON
            CPI       '0'
            JRNZ      BA2
            DCR       D
            JRNZ      BA3
BA2:        MOV       M,B
            INX       H
BA3:        MOV       A,E
            ADI       '0'
            MOV       M,A
            INX       H
            RET
TCON:       MVI       B,2FH
            INR       B
            SUB       C
            JRNC      TCON+2
            ADD       C
            MOV       E,A
            MOV       A,B
            RET
;
;
SETHW:      LDA       HO
```

```
            OUT      T0
            LDA      H1
            OUT      T1
            LDA      H2
            OUT      T2
            RET
;
;
MONTH:      LDA      MON
            MVI      D,0
            MOV      E,A
            LXI      B,MONT
            XCHG
            DAD      B
            XCHG
            MVI      B,17
            JMPR     BLT         ; RETURN FROM THERE
;
;
;
;          ·**** BLOCK TRANSFER ****
;
;....SOURCE: <DE> ....DEST: <HL> ....LENGTH: <B> ....
;
BLT:        LDAX     D                        ; GET CHAR
            MOV      M,A                       ; MOVE IT
            INX      H                         ;
            INX      D
            DCR      B
            JRNZ     BLT
            RET
;
;
;          **** CLEARING A BLOCK OF MEMORY ****
;          ****    OR SETTING A BLOCK TO ' ' ****
;
SETBLK:     MVI      A,20H
            JMPR     CLRB2
CLRBLK:     MVI      A,NUL
CLRB2:      MOV      M,A
            INX      H
            DCR      B
            JRNZ     CLRB2
            RET
;
;
;          **** OUTPUTTING A STRING ****
;
OUTSTR:     LDAX     D                        ; GET CHARACTER
            CPI      '$'
            RZ
            CALL     OUCH
            INX      D
            JMPR     OUTSTR
;
;
;                 *** OUTPUTTING STRING + <CR><LF> ***
;
OUST:       CALL     OUTSTR
            JMPR     CRLF
```

```
;
;
;          *** OUTPUTTING A NUMBER FROM PROMPT ****
;
NUMBER:  LDA      SEE
         INR      A
         STA      SEE
         ADI      2FH       ; LET OUCH DO THE REST
;
;
;          **** OUTPUTTING A CHARACTER ****
;
OUCH:    PUSH     PSW
         IN       STAT
         ANI      1
         JRZ      OUCH+1
         POP      PSW
         OUT      DAT
         RET
;
;
;          **** INPUTTING A CHARACTER ****
;
INCH:    IN       STAT
         ANI      2H
         JRZ      INCH
         IN       DAT
         ANI      7FH
         CPI      STAT      ;©C
         RNZ
         JMP      NUL       ; REBOOT
;
;
;          **** INPUT OUTPUT W/ECHO ****
;
ECHO:    CALL     INCH
         JMPR     OUCH
;
;
;          **** <CR><LF> ****
;
CRLF:    MVI      A,CR
         CALL     OUCH
         MVI      A,LF
         JMPR     OUCH
;
;
;          **** INPUTTING A NUMBER STRING ****
;                 *** N<=64K ***
;          **** RESULT LEFT IN HL PAIR ****
;
INUM:    LXI      H,NUL
INLP:    CALL     ECHO
         CPI      CR
         RZ
         SBI      30H
         RM                           ; WON'T WORK IF < '0'
         CPI      0AH                 ; N > 9  ???
         JM       INLP2               ; NOPE..IT'S GOOD
         XRA      A                   ; CLEAR IT
```

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```
        DCR     A                       ; SET NEGATIVE
        RET
INLP2:  LXI     D,NUL
        DAD     H
        XCHG
        DAD     D
        DAD     H
        DAD     H
        XCHG
        DAD     D
        MVI     D,NUL
        MOV     E,A
        DAD     D
        JMPR    INLP
;
;
;
;       **** INPUTTING DATA ****
;
;
INPT:   LXI     D,MSG12         ; <CR> WHEN READY
        CALL    OUST
        CALL    ECHO
        CPI     STAT            ; ©C ??
        JZ      NUL             ; JUMP TO CPM
        CPI     CR
        JRNZ    INPT
        LXI     H,RAN1  ; TWO CHANNELS
        LDA     CNT
        DCR     A
        JRNZ    INSKP   ; MUST BE TWO
        LXI     H,RANO
INSKP:  SHLD    JMPVCT
        CALL    INCHEK
        MVI     A,BELL                  ; DING DONG
        CALL    OUCH
RADM:   CALL    TICK            ; PAUSE ONE CLOCK TICK
        CALL    INSTEP          ; CHECK FOR ABORT
        LHLD    JMPVCT
        PCHL    ; JMP FROM HERE
RAN1:   LXI     H,CST1
        CALL    TIME
        JRNC    RANO
        LHLD    SHL1
        MVI     A,1
        CALL    ADAV
        SHLD    SHL1
RANO:   LXI     H,CSTO
        CALL    TIME
        JRNC    RADM
        LHLD    SHLO
        MVI     A,0
        CALL    ADAV
        SHLD    SHLO
        LDA     SEE
        ORA     A
        CNZ     MONIT
        LDA     SIZE
        DCR     A
        STA     SIZE
```

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```
        JRZ     HISIZ
        CPI     OFFH
        JRNZ    RADM
        LDA     SIZE+1
        DCR     A
        STA     SIZE+1
        JMPR    RADM
HISIZ:  LDA     SIZE+1
        ORA     A
        JRNZ    RADM
        CALL    STEP    ; ADVANCE
        LHLD    SIZES   ; RESET BLOCK SIZE
        SHLD    SIZE
        LDA     NUMBLK
        DCR     A
        STA     NUMBLK
        JRZ     HISTP
        CPI     OFFH
        JRNZ    RADM
        LDA     NUMBLK+1
        DCR     A
        STA     NUMBLK+1
        JMPR    RADM
HISTP:  LDA     NUMBLK+1
        ORA     A
        RZ
        JMPR    RADM
;
;
;
;
;       **** STEPPING MOTOR AHEAD ****
;
STEP:   LHLD    STEPS    ; GET # STEPS
        XCHG
STLP:   CALL    STP
        DCX     D
        MOV     A,E
        ORA     D
```

```
        JRNZ    STLP
        RET
;
;
;       *** LEAP BACKWARD ***
;
LPBACK: LXI     D,1000H ; 400 NUMBERS
SBLP:   CALL    BSTP
        DCX     D
        MOV     A,E
        ORA     D
        JRNZ    SBLP
        RET
;
;
;       **** STEP MOTOR ONE STEP BACKWARD ****
;
BSTP:   PUSH    B
        MVI     B,2
STPLPB: MVI     A,0
        CALL    POUT
        MVI     A,2
        CALL    POUT
        MVI     A,0
        CALL    POUT
        DCR     B
        JRNZ    STPLPB
        POP     B
        RET
;
;
POUT:   OUT     0          ; MOTOR LOC'N
WAIT:   PUSH    B                    ; SAVE IT
        LXI     B,02H
WTLP:   DCR     B
        JRNZ    WTLP
        DCR     C
        JRNZ    WTLP
        POP     B
        RET
;
;
;
;
;       **** STEPPING FORWARD ****
;
STP:    PUSH    B
        MVI     B,2
STPLPF: MVI     A,4H
        CALL    POUT
        MVI     A,6H
        CALL    POUT
        MVI     A,4H
        CALL    POUT
        DCR     B
        JRNZ    STPLPF
        POP     B
        RET
;
;
```
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```
;          **** ZERO-ING START LOCATION ****
;
ZERO:     CALL      INCH                ; GET CMD
          CPI       'B'                 ; BACK OPE STEP
          JRZ       ZBACK
          CPI       'L'                 ; LEAP BACK
          JRZ       ZLEAP
          CPI       'F'                 ; ONE STEP FORWARD
          JRZ       ZFORW
          CPI       'J'                 ; JUMP FORWARD
          JRZ       ZJUMP
          CPI       CR
          JRZ       ZEND
          MVI       A,BELL
          CALL      OUCH
          JMPR      ZERO
ZBACK:    CALL      BSTP
          JMPR      ZERO
ZLEAP:    CALL      LPBACK
          JMPR      ZERO
ZFORW:    CALL      STP
          JMPR      ZERO
ZJUMP:    LXI       D,1000H
          CALL      STLP
          JMPR      ZERO
ZEND:     DCR       A           ; NON-ZERO RETURN
          RET
;
;
;          **** RETURN TO ORIGINAL START ****
;
RTURN:    LHLD      NUMBLK+2
          INX       H           ; CORRECT IT
TRTLP:    XCHG
          LHLD      STEPS
          XCHG
          CALL      SBLP
          DCX       H
          MOV       A,L
          ORA       H
          JRNZ      TRTLP
          LXI       D,500H
          CALL      SBLP
          LXI       D,500H
          JMP       STLP
;
;
;          **** CHECKING FOR INPUT ****
;
INCHEK:   CALL      INSTEP
          XRA       A
          CALL      ADDRIV
          XRA       A                   ; SET TO 0
          ADD       E                   ; ANYTHING ??
          RNZ
          ADD       D                   ; OR HERE ??
          JRZ       INCHEK              ; NOPE
          RET
;
;
```

```
;       **** ©C ABORT CHECK ****
;
INSTEP: IN      STAT
        ANI     DAT
        RZ
        IN      DAT
        ANI     7FH
        CPI     03H       ; ©C
        RNZ
        JMP     NUL       ; ABORT TO CPM
;
;
;       **** COMPUTING STEPS PER 'TIC' ****
;
SETSTP: XRA     A         ; CLEAR CARRY
        MOV     A,H       ;
        RLC               ; LEFT INTO CARRY
        MOV     D,A       ; RESULT TO DE
        MOV     A,L
        RLC
        MOV     E,A
        RET
;
;
;       **** COMPUTING SAMPLE INTERVAL TIMES ****
;
SETIM:  MOV     A,H                    ; COMPLIMENT TO BC PAIR
        CMA
        MOV     B,A
        MOV     A,L
        CMA
        MOV     C,A
        INX     B                      ; ..DONE COMPLIMENTING
        LXI     H,MAX                  ; 300/SEC
        LXI     D,NUL                  ; CLEAR BC PAIR
SETLP:  DAD     B
        MOV     A,H
        ORA     A
        RM                             ; RESULT LEFT IN <DE>
        INX     D
        JMPR    SETLP
;
;
;       **** COMPUTES ELAPSED TIME ****
;
TICK:   IN      6
        ANI     4H
        JRZ     TICK
        MVI     A,50H
        OUT     6
        RET
;
;
;
TIME:   MOV     A,M
        DCR     A
        MOV     M,A
        JRZ     HITIM
        CPI     0FFH      ; UNDERFLOW ??
        JRNZ    GOODT     ; NO CARRY..NO ZERO
```

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```
        INX    H
        MOV    A,M
        DCR    M
        RET
HITIM:  INX    H
        MOV    A,M
        ORA    A
        RNZ                 ; ZERO..NO CARRY
        PUSH   D
        MOV    E,L
        MOV    D,H
        INX    H
        INX    H            ; LOOK AT SAVED COPY
        MOV    A,M
        STAX   D
        DCX    H
        DCX    D
        MOV    A,M
        STAX   D
        POP    D
        STC                 ; SET CARRY
        RET
GOODT:  XRA    A            ; CLEAR EVERYTING
        RET
;
;
;                 **** MONITORING INPUT ****
;
MONIT:  MVI    A,20H    ; SPACE
        CALL   OUCH
        CALL   OUCH
        CALL   OUCH
        MOV    A,D
        CALL   CNVERT
        MOV    A,E
        CALL   CNVERT
        MVI    A,CR
        JMP    OUCH
;
;
;                 **** MOVING CONVERSIONS TO MEM ****
;
ADAV:   PUSH   H
        LXI    H,NUL
        MVI    B,20H             ; = 32
ADLP2:  PUSH   PSW               ; COLLECT 32 SAMPLES
        CALL   ADDRIV
        POP    PSW
        DAD    D
        DCR    B
        JRNZ   ADLP2             ; END OF SAMPLES
        MVI    B,5H              ; 2**5 = 32
ADLP3:  XRA    A                 ; DIVIDING BY 32
        MOV    A,H
        RAR
        MOV    H,A
        MOV    A,L
        RAR
        MOV    L,A
        DCR    B
```

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```
        JRNZ      ADLP3              ; END OF DIVISION
        XCHG
        POP       H                  ; SAVE RESULT
        MOV       M,D
        INX       H
        MOV       M,E
        INX       H
        RET
;
;
;                 **** A TO D DRIVER ****
;
ADDRIV: OUT       DSTAT
        NOP
ADLP1:  IN        DSTAT
        RRC
        JRC       ADLP1
        IN        DDAT
        MOV       E,A
        IN        DDAT
        ANI       03H
        MOV       D,A
        RET
;
;
;
;                 *** SAVE THE FILENAME ***
;
SAVEFN: LXI       H,SAVFIL           ; DESTINATION
        LXI       D,FCB              ; SOURCE
        MVI       B,11               ; FILENAME + EXT
        JMP       BLT                ; TRANSFER & RET
RESTFN: LXI       D,SAVFIL           ; SOURCE
        LXI       H,FCB              ; DESTINATION
        MVI       B,11
        JMP       BLT
;
;
;
;
;
;                 **** BDOS DRIVERS ****
;
DMAKE:  LXI       D,FCB
        MVI       C,CREATE
        CALL      BDOS
        RET
;
;
DOPEN:  LXI       D,FCB
        MVI       C,OPEN
        CALL      BDOS
        RET
;
;
DWRIT:  LXI       D,FCB
        MVI       C,WRITE
        CALL      BDOS
        RET
;
```

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```
;
DCLOS:   LXI     D,FCB
         MVI     C,CLOSE
         CALL    BDOS
         RET
;
;
DFIND:   XRA     A
         STA     TEMP     ; CLEAR TEMP
         LDA     CNT
         STA     TEMP2    ; GET # OF CHANNELS
         CALL    SAVEFN   ; SAVE THE FILENAME
DFLP:    LXI     D,FCB
         MVI     C,FIND
         CALL    BDOS
         INR     A
         CNZ     SETEMP   ; NONZERO = FILE FOUND
         CALL    UPFILE   ; UPDATE FILENAME
         LDA     TEMP2    ; GET COUNT
         DCR     A
         STA     TEMP2
         JRNZ    DFLP     ; STILL MORE TO CHECK
         CALL    RESTFN   ; RESTORE FILENAME
         LDA     TEMP     ; FOUND STATUS...0= NONE FOUND
         DCR     A        ; -1 = NON FOUND
         RET
;
;
;
SETEMP:  MVI     A,DAT    ; NON ZERO
         STA     TEMP     ; SET IT
         RET
;
;
;
DERASE:  CALL    SAVEFN
         LDA     CNT
         STA     TEMP2
RASLP:   CALL    CLRFN    ; START FRESH
         LXI     D,FCB
         MVI     C,ERASE
         CALL    BDOS
         CALL    UPFILE
         LDA     TEMP2
         DCR     A
         STA     TEMP2
         JRNZ    RASLP    ; ERASE THE NEXT ONE
         CALL    RESTFN   ; RESTORE THE FILENAME
         RET
;
;
;            **** INIT MEM LOC'S ****
;
INIT:    XRA     A
         OUT     0        ; TURN OFF MOTOR
         LXI     H,SHLO
         LXI     D,START0
         CALL    SAVEN
         LXI     D,START1
         JMP     SAVEN
;
```

```
;
;          **** ERROR EXITS AND MSG CALLS ****
;
CRERR:    LXI       D,ERRM1
          JMPR      ERRQ
FLERR:    LXI       D,ERRM2
          JMPR      ERRQ
WRER:     LXI       D,ERRM3
          JMPR      ERRQ
MSCER:    LXI       D,ERRM4
ERRQ:     CALL      OUST
          MVI       A,BELL              ; DINGALING
          CALL      OUCH
          JMP       NUL
;
;
;
;
;
UNI:      .BYTE     0
CNT:      .BYTE     0
NUM:      .BYTE     0
SEE:      .BYTE     0
SLOW:     .BYTE     0
OFST:     .BYTE     0
BLKSZ:    .BYTE     0
H0:       .BYTE     0
H1:       .BYTE     0
H2:       .BYTE     0
HH:       .BYTE     0
MM:       .BYTE     0
SS:       .BYTE     0
TEMP:     .BYTE     0
TEMP2:    .BYTE     0
JMPVCT:   .WORD     0
TXTSZ:    .WORD     0
TXTSZ2:   .WORD     0
CST0:     .WORD     0
CSTS0:    .WORD     0
CST1:     .WORD     0
CSTS1:    .WORD     0
SIZE:     .WORD     0              ; SAMPLES/BLOCK
SIZFS:    .WORD     0
NUMBLK:   .WORD     0,0            ; #BLOCKS/RUN
STEPS:    .WORD     0,0            ; STEPS BETWEEN BLOCKS
SHL0:     .WORD     0
SHL1:     .WORD     0
SIZ0:     .WORD     0
SIZ1:     .WORD     0
C8600:    .BYTE     128,81,1
C3600:    .BYTE     16,14,0
C60:      .BYTE     60,0,0
C1:       .BYTE     1,0,0
SAVFIL:   .BLKB     12
MON:      .BYTE     85
MONT:     .ASCII    ® JANUARY    1982    ®      ; 0
MON2:     .ASCII    ® FEBRUARY   1982    ®      ; 17
MON3:     .ASCII    ® MARCH    1982    ®        ; 34
MON4:     .ASCII    ® APRIL    1982    ®        ; 51
MON5:     .ASCII    ® MAY  1982        ®        ; 68
```

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MON6:    .ASCII   ® JUNE    1981      ®      ; 85
MON7:    .ASCII   ® JULY    1981      ®      ; 102
MON8:    .ASCII   ® AUGUST   1981     ®      ; 119
MON9:    .ASCII   ® SEPTEMBER 1981    ®      ; 136
MON10:   .ASCII   ® OCTOBER   1981    ®      ; 153
MON11:   .ASCII   ® NOVEMBER   1981   ®      ; 170
MON12:   .ASCII   ® DECEMBER   1981   ®      ; 187
SMPSC:   .ASCII   ® SAMPLES.   SAMPLE PERIOD = ®
CLKDT:   .ASCII   ® TIMES 3.3280 MSEC
®
DMSG:    .ASCII   ® SAMPLES/BLK ; ®
DM2:     .ASCII   ® BLKS/RUN
®
MSGA:    .ASCII   ®
         REVERSE         FORWARD

STEP:    'B'             'F'
JUMP:    'L'             'J'


....TO EXIT :   <CR>   : ? $®
MSGB:    .ASCII   ®
TO RESET START POINT...<CR>
   ELSE ...<SPACE>  : ? $®
MSG4:    .ASCII   ®
UNI- OR BI-POLAR ? (U OR B) : $®
MSG5:    .ASCII   ®
SET SWITCH TO LEFT (U)®
MSG6:    .ASCII   ®
ADJUST RIGHT POT FOR "0000" (END W/<CR>)$®
MSG7:    .ASCII   ®
ADJUST LEFT POT FOR "01FF"$®
MSG8:    .ASCII   ®
SET SWITCH TO THE RIGHT (B)®
MSG9:    .ASCII   ®
ADJUST CENTER POT FOR "0200" (END W/<CR>)$®
MSG10:   .ASCII   ®
ADJUST LEFT POT FOR "03FF"$®
MSGF:    .ASCII   ®
FILE(S) ALREADY ON DISK....RENAME NEW FILE ? $®
MSGQ:    .ASCII   ®
NEW FILENAME(.EXT) : $®
MSGW:    .ASCII   ®
OLD FILE(S) WILL BE DESTROYED...ARE YOU SURE ? $®
MSGS:    .ASCII   ®
FAST OR SLOW MONITOR ?? (F=9600,S=300) : $®
ERRM1:   .ASCII   ®
CANNOT CREATE FILE....
®
ERRM2:   .ASCII   ®
FILE ERROR.....
$®
ERRM3:   .ASCII   ®
WRITE ERROR ON DISK $®
ERRM4:   .ASCII   ®
?????$®
MSG12:   .ASCII   ®
TYPE A <CR> WHEN READY.®
MSG14:   .ASCII   ®
ABORT BY TYPING A <®C> $®
MSGR:    .ASCII   ®
```

```
WANT TO TAKE MORE DATA (Y OR N ) : $®
MSGT:     .ASCII   ®
WANT TO MONITOR INPUT ? (Y OR N) : $®
MSGP:     .ASCII   ®
COLLECTION COMPLETE..PLEASE WAIT$®
MSGL:     .ASCII   ®
ONE LINE FOR INPUT >>>® [BELL]
MSGL2:    .ASCII   ®
<CR> ENDS ... <ESC> RESETS ... <RUBOUT> DELETES $®
MSG:      .ASCII   ®
# OF CHANNELS (1-2): $®
MSG0:     .ASCII   ®
SAMPLES PER BLOCK (CHAN 0) : $®
MSG1:     .ASCII   ®
BLOCKS PER RUN : $®
MSG2:     .ASCII   ®
SAMPLES PER SECOND ? (100 MAX) CHAN(#0) :$®
MSGE:     .ASCII   ®
SAMPLES PER SECOND ? (100 MAX) CHAN(#1) :$®
MSG3:     .ASCII   ®
STEPS BETWEEN BLOCKS : $®
TXTBUF: .BLKB    80H        ; TEXT BUFFER
;
;
NUL        ==        00H
DAT        ==        2H
STAT       ==        3H
BELL       ==        07H
CR         ==        0DH
LF         ==        0AH
DSTAT      ==        41H
DDAT       ==        40H
MAX        ==        012CH
T0         ==        0FCH
T1         ==        T0+1
T2         ==        T0+2
TT         ==        H()
DD         ==        0FFFH
M10000     ==        0D8F0H
TTHOU      ==        10000
M1000      ==        0FC18H
THOU       ==        1000
M100       ==        0FF9CH
HUND       ==        100
M10        ==        0FFF6H
TEN        ==        10
START0     ==        1000H
OFF0       ==        10H
START1     ==        9000H
OFF1       ==        90H
;
;
;
;                    **** BDOS EQUATES ****
;
BDOS       ==        05H
OPEN       ==        15        ; -1 IF NOT FOUND
WRITE      ==        21        ; 0=SUCCESS
                               ; 1=ERROR IN EXTENDING
                               ; 2=NO MORE ROOM
```

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```
CLOSE    ==      16          ; -1 IF NOT PRESENT
ERASE    ==      19
CREATE   ==      22          ; -1 = NO DIRECTORY SPACE AVAIL
FIND     ==      17          ; -1 IF NOT FOUND
BUFF     ==      80H
FCB      ==      5CH
FCBN     ==      FCB
FCBFN    ==      FCB+1       ; NAME
FCBEX    ==      FCB+9       ; EXT
;
;
         .END    BEGIN
```

00000000000000000000000000000000
  000000000000000000000000000000
  000000000000

APPENDIX B

APPENDIX B

```
C
C       OZONE.FOR
C
C       THIS PROGRAM ACCEPTS Z-80 GENERATED ADC FILES
C       ORIGINATING FROM DATA TAKEN ON A PERKIN-ELMER
C       DOUBLE BEAM SPECTROPHOTOMETER AND PLOTS EITHER
C       TRANSMISSION OR
C       ABSORPTION COEFFICIENTS VRS. WAVELENGTH OR ENERGY
C
C

        COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
        COMMON/PLOT/NPS,XMIN,XMAX,YMIN,YMAX,XGPON,,YGPON,
       1XGPOX,YGPOX,NUPAGE,NUGRAF,LNTYP,ISTP,ISYM,IXSCL,
       1IYSCL,IT
        DIMENSION Y(6500),TIT1(59),TIT2(59),YB(6500)
        DIMENSION XA(6500),XDAT(6500),YDAT(6500)
        DIMENSION TIT3(59),TIT4(59),TIT5(59)
        EQUIVALENCE  (YDAT,YB)
        DOUBLE PRECISION FNAME,BNAME
        DATA TIT1/'E','N','E','R','G','Y',' ','('
       1,'E','V',')',48*' '/
        DATA TIT2/'A','B','S','O','R','P','T','I','O','N'
       1,49*' '/
        DATA TIT3/'T','R','A','N','S','M','I','S','S
       1','I','O','N',47*' '/
        DATA TIT4/'W','A','V','E','L','E','N','G','T','H'
       1,' ','(','A','N','G','S','T','R','O','M','S',')'
       1,37*' '/
C
        DATA TIT5/'W','A','V','E','N','U','M','B','E',
       1'R',' ','(','C','M','-','1',')',42*' '/
C
C
68      TYPE 78
78      FORMAT(1X/1X'PLOT TRANSMISSIONS(1) ABSORP. COEF.
       1(2) INDUCED ABSORB.(3) DIFFERENCE(4)?:'$)
        ACCEPT *, PLOT
        NORM=0
        IF(PLOT.EQ.1.OR.PLOT.EQ.2.OR.PLOT.EQ.4) GO TO 1000
        TYPE 15
15      FORMAT (1X,/1X,'TYPE IN PRE-IRRAD. FILE NAME:'$)
        ACCEPT 6, BNAME
        CALL READ(YB,BNAME)
1000    TYPE 5
5       FORMAT (' TYPE IN FILE NAME:'$)
        ACCEPT 6, FNAME
6       FORMAT (A10)
        CALL READ(Y,FNAME)
```

```
          IF(PLOT.EQ.4) TYPE 5
          IF(PLOT.EQ.4) ACCEPT 6, FNAME
          IF(PLOT.EQ.4) GO TO 664
          TYPE 18
18        FORMAT(1X/1X'NORMALIZE ? FILENAME?')
          ACCEPT *, NORM
          IF(NORM.EQ.1) ACCEPT 6, BNAME
664       IF(NORM.EQ.1) CALL READ(YB,BNAME)
          IF(PLOT.EQ.4) CALL READ(YB,FNAME)
          IF(NORM.NE.1) GO TO 82
          DO 66 IJ=1,NPTS
          IF(YB(IJ).LE.0.80) YB(IJ)=YB(IJ-1)
66        Y(IJ)=Y(IJ)/YB(IJ)
82        IF(PLOT.EQ.4) CALL DIFF(Y,YB)
          IF(PLOT.EQ.1.OR.PLOT.EQ.4) GO TO 2000
          IF(PLOT.EQ.2) GO TO 1001
          CALL INDABS(Y,YB)
          GO TO 3
1001      CALL ABSORP(Y)
     3    CONTINUE
2000      TYPE 300
300       FORMAT(1X/1X'SMOOTH DATA N TIMES..ENTER N')
          ACCEPT *, NSMOOT
          IF(NSMOOT.EQ.0) GO TO 301
          DO 17 I=1,NSMOOT
17        CALL SMOOTH(Y,NPTS)
301       NUPAGE='YES'
          NUGRAF='YES'
          IXSCL=1
          IYSCL=1
224       XGPON=1.
          YGPON=1.
          XGPOX=7.5
          YGPOX=5.5
          XHLPOS=2.75
          YHLPOS=.25
          XVLPOS=0.
          YVLPOS=5.0
          IT=5
911       TYPE 173
173       FORMAT(1X/1X'YMIN,YMAX ?')
          ACCEPT *, YMIN,YMAX
          TYPE 177
177       FORMAT(1X/1X'X-AXIS: ENERGY(EV) (1), WAVELENGTH
(2),
     1WAVENUMBER (3) ?:'$)
          ACCEPT *, NIX
          CALL XCALIB(XA,NIX)
          TYPE 189
189       FORMAT(1X/1X'ENTER XMIN XMAX')
          ACCEPT *, XMIN,XMAX
178       LNTYP=-4
          ISTP=1
          ISYM=0
          L1=1
```

```
          TYPE 70
70        FORMAT(1X/1X'TAKE EVERY --TH POINT')
          ACCEPT *, NSKIP
          DO 62 K=1,NPTS,NSKIP
          XDAT(L1)=XA(K)
          YDAT(L1)=Y(K)
   62 L1=L1+1
          NPS=L1-1
188           CALL PLTGEN(XDAT,YDAT)
          IF(NIX.EQ.2) CALL LABL(XHLPOS,YHLPOS,'H',TIT4,0.)
          IF(PLOT.EQ.1) CALL LABL(XVLPOS,YVLPOS,'V',TIT3,0.)
          IF(NIX.EQ.1) CALL LABL(XHLPOS,YHLPOS,'H',TIT1,0.)
          IF(PLOT.EQ.2) CALL LABL(XVLPOS,YVLPOS,'V',TIT2,0.)
          IF(NIX.EQ.3) CALL LABL(XHLPOS,YHLPOS,'H',TIT5,0.)
          NUPAGE='NO'
          NUGRAF='NO'
   67 CONTINUE
          CALL MOVABS(600,710)
          CALL ANMODE
          TYPE 1234, FNAME
1234      FORMAT(1XA10)
          CALL TINPUT(KL)
          CALL ERASE
          NUPAGE='YES'
          NUGRAF='YES'
          TYPE 142
142       FORMAT(1X/1X'GRAPH AGAIN ?')
          ACCEPT *, GRAG
          IF(GRAG.EQ.1) GO TO 911
          TYPE 63
   63 FORMAT (1X/' CHOOSE ANOTHER FILE? YES(1) NO(0)'/)
          ACCEPT 2, IANS
2         FORMAT(I5)
          IF (IANS.EQ.1) GO TO 68
          CALL EXIT
          END
C
C
C
          SUBROUTINE INDABS(Y,YB)
          COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
          DIMENSION Y(1),YB(1)
          TYPE 16
   16 FORMAT (1X/1X,'THICKNESS OF SAMPLE (IN CM)'/)
          ACCEPT *, T
          T=1/T
   44 DO 4 K=1,NPTS
   11 XX=1/Y(K)
          TD2=XX**2
          Y(K)=ALOG(XX)
          Y(K)=T*Y(K)
          XX1=1/YB(L)
          TB2=XX1**2
          XX2=ALOG(XX1)
          XX2=T*XX2
```

```
          Y(K)=Y(K)-XX2
      4   CONTINUE
          RETURN
          END
C
C
C

          SUBROUTINE READ(Y,FNAME)
          COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
          DIMENSION Y(1),N(6500)
          DOUBLE PRECISION FNAME
          TYPE 100
100       FORMAT(1X/1X'SUBROUTINE READ')
          OPEN(UNIT=23,FILE=FNAME)
          READ(23,*) NMBLKS,NSPB,NPTS,START,STOP
          READ(23,200) (N(K),K=1,NPTS)
200       FORMAT(8(I4,1X))
          DO 10 I=1,NPTS
          Y(I)=N(I)/1023.
10        CONTINUE
          CLOSE(UNIT=23,FILE=FNAME)
          RETURN
          END
C
C
C

          SUBROUTINE XCALIB(X,NIX)
          COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
          DIMENSION X(1)
   TYPE 500
500          FORMAT(1X/1X'SUBROUTINE XCALIB')
          DO 4 K=1,NPTS
          ZIP=START-FLOAT(K)*(START-STOP)/NPTS
          XX3=ZIP*1.0E-8

IF(NIX.EQ.1)X(K)=((2.9979E10/XX3)*6.6256E-27)/1.6E-12
          IF(NIX.EQ.2) X(K)=ZIP
          IF(NIX.EQ.3) X(K)=1./XX3
      4   CONTINUE
          RETURN
          END
C
C
C

          SUBROUTINE ABSORP(Y)
          COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
          DIMENSION Y(1)
          TYPE 77
77        FORMAT(1X/1X'BASE 10(1) OR BASE E(2) ?:'$)
          ACCEPT *,BASE
          TYPE 16
     16   FORMAT (1X/1X,'OPTICAL PATH LENGTH (IN CM):'$)
          ACCEPT *, T
          T=1/T
          TYPE 22
```

```
22      FORMAT(1X/1X'ENTER TEMP(KELVIN) AND
PRESSURE(CM):'$)
        ACCEPT *, TEMP ,SP
        STP=76*TEMP/(SP*273)
    44 DO 4 K=1,NPTS
        IF(Y(K).LE.0.0) Y(K)=Y(K-1)
    11 XX=1/Y(K)
        IF(BASE.EQ.1) GO TO 66
        Y(K)=STP*T*ALCG(XX)
        GO TO 4
66      Y(K)=STP*T*ALOG10(XX)
     4 CONTINUE
        RETURN
        END
C
C
C
        SUBROUTINE DIFF(Y,YB)
        COMMON/PARAM/NPTS,T,NMBLKS,NSPB,START,STOP
        DIMENSION Y(1),YB(1)
  FRAC=76./273.
        TYPE 10
10      FORMAT(1X/1X'SUBROUTINE DIFF')
        TYPE 20
20      FORMAT(1X/1X'ENTER P1,T1 AND P2,T2:'$)
        ACCEPT *, P1,T1,P2,T2
        TYPE 60
60      FORMAT(1X/1X'ENTER OPTICAL PATH LENGTH (CM):'$)
        ACCEPT *, T
        T=1./T
        DO 11 I=1,NPTS
        ARG=(YB(I)**(T2/P2) / Y(I)**(T1/P1))
        Y(I)=ALOG10(ARG)*T*FRAC
11      CONTINUE
        RETURN
        END
```